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Elastic and inelastic scattering of conduction electrons from oscillating impurities in semiconductors

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ELASTIC AND INELASTIC SCATTERING OF CONDUCTION ELECTRONS FROM OSCILLATING IMPURITIES IN SEMICONDUCTORS

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To Professors D. G. Frood and V. V. Paranjape

and

To Drs. A. Oguchi and P. Lal

and

To My Parents

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ABSTRACT

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Elastic scattering and inelastic scattering of conduction electrons by oscillating ionized impurities in semiconductors have been analyzed on the assumption that the scattering potential is the Coulomb potential between the conduction electrons and the excess charge of the impurity ions and that the electrons are non-degenerate and have a simple spherical energy bands. Two possible cases for impurity oscillations by thermal agitation are considered; (i) ionized impurities oscillating with a localized oscillating frequency, ω_o, widely separated from the normal acoustic and optical modes of the crystal, and (ii) ionized impurities oscillating with frequencies common to those of host lattice.

The analysis shows that the effect of impurity oscillation tends to increase the effective deformation potential coupling constant, and hence to decrease the effective electron-phonon relaxation time. But the change of those parameters due to this effect is very small in most extrinsic semiconductors even at temperatures up to their melting point and with impurity concentrations reaching the degenerate condition. The computed results including the effect of impurity oscillation are practically similar to those of Conwell and Weisskopf, and Brooks and Herring. This effect can not explain the deviation from the $T^{3/2}$ law experimentary observed in several semiconductors such as Ge and Si.

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INTRODUCTION

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In valence semiconductors it is well-known that the formula of Conwell and Weisskopf (1950) accounts reasonably well for mobility arising from the scattering of electrons from ionized impurities. In this model the impurities are assumed to be stationary and the electron (n-type semiconductors) or the hole (p-type semiconductors) are scattered elastically from a fixed Coulomb field. This formula leads to a $T^{3/2}$ temperature dependence of the electric mobility. There are, however, many examples of semiconductors with mobility dominated by ionized impurity scattering, where deviation from the $T^{3/2}$ law has been observed (see, e.g., Debye and Conwell (1954); Morin and Maita (1954); Ludwing and Watters (1956)). These experimental evidences show that a temperature dependence of the mobility generally follows the form T^n with $\frac{1}{2} \leq n \leq 2\frac{1}{2}$.

Many investigators have considered the effects to be expected in a medium containing a number of impurities. Brooks (1951) replaced the Coulomb potential by a potential screened by the conduction electrons and obtained essentially the same result as obtained by Conwell and Weisskopf (1950), who used a simple Rutherford scattering law, as for an unscreened ionized impurity, but cut off the scattering at small angles. Dingle (1955) considered these problems in detail. Horie (1950) took into account the local dilatation of the lattice in the neighbourhood of the impurity center.

It is actually not easy to account for the departures of the impurity mobility from the $T^{3/2}$ law. These theories are affected in only the cut-off effect in the scattering cross section and this quantity enters logarithmically into the expression for the mobility, so that this effect is rather weak. In most circumstances it does not seriously modify the temperature dependence from that given by Conwell and Weisskopf (1950). Another possible correction is that for electron-electron collisions which act to equalize the distributions, and hence reduce the mobility (Spitzer and Harm (1955)).

To explain the observed temperature dependence of the properties of a semiconductor, we shall consider more closely some of the mechanisms that scatter electrons in crystals. The two most significant modes are scattering by ionized impurities and scattering by thermal oscillations of a crystal. These scattering mechanisms occur simultaneously in real crystals. We shall consider the effects of elastic scattering by ionized oscillating impurities in Parts I and II, and the effects of inelastic scattering by ionized oscillating impurities in Part III, where we shall derive the effective deformation potential (the electron-phonon coupling) constant, $C_{eff}(T,n_D^{(+)})$, by comparison with the ordinary lattice-electron scattering result for a pure crystal (Kittel (1963)) to see the effects of the temperature, T, and the ionized oscillating impurity density, $n_D^{(+)}$. We shall derive the relaxation time from which we can deduce the various transport coefficients.

We introduce in this thesis a model in which the impurity atom oscillates around a fixed equilibrium position. This kind of model was first introduced by Koshino (1960, 1963) to understand departures of the resitivity of dilute alloys from Matthiessen's rule. Similar investigation was made by Taylor (1962, 1964). That impurity atoms are oscillating around their equilibrium positions is self-evident and the conduction electrons are scattered by not only host atoms but impurity atoms. Hence the scattering from localized ionized oscilating impurity atoms or from ionized oscillating impurity atoms incorporated with the host atoms may contribute the electronic conduction significantly. We therefore consider the following two possible cases.

In Part I, we consider the impurity to have a localized oscillating frequency, ω_o , widely separated from the normal acoustic and optical modes of the crystal. This model implies that the frequency, ω_o , is larger than $k_B\Theta/\hbar$ where Θ is the Debye temperature of the crystal. For simplicity we treat the ionized impurity atom as a simple harmonic oscillator which scatters the conduction electron through an oscillating Coulomb force field. We introduce a cut-off equal to the half distance between impurity centres to avoid the divergence of the Coulomb type cross section.

In Parts II and III, we consider a more developed model in which the ionized impurity atoms oscillate with frequencies common to those of the host atoms. We assume here that the thermal motion of ionized impurity atoms is identical with that of the host atoms.

This assumption may be valid particularly at low acoustic frequencies since for long wave lengths many atoms are moving in the same direction and will carry the impurities with them when the mass and the valence of the impurity atoms are not much different from those of the host atoms.

The problem here is thus one of normal modes and we consider the phonon absorption or emission process due to the thermal motion of ionized impurity atoms interacting with the conduction electron through an oscillating, screened Coulomb force field, where electron-lattice interaction involves the absorption or emission of one or more acoustic phonons and hence such processes are inelastic. However, the cross section for an electron scattering from ionized oscillating impurity atoms has also an elastic part in which no acoustical phonons are absorbed or emittted. We thus consider the full elastic scattering processes as well as the inelastic scattering process for the cross section of the oscillating, screened **Coulomb field**.

The relaxation time due to the full elastic part is obtained by the theory mathematically identical with that for the recoil-free γ-ray emission by nuclei bound in solids (Mössbauer (1958)) or that of newtron capture by crystals (Lamb (1939)) and also with that of X-ray scattering from a crystal; the well-known Debye–Waller effect (see, e.g., Ziman (1972)).

The relaxation time due to the inelastic part is derived by solving the Boltzmann transport equation (see, e.g., Wilson (1965)).

PART I

Electron Scattering from Localized Oscillating Impurities

1. Model Hamiltonian

To determine the relaxation time due to scattering of conducton electrons by ionized impurity atoms in semiconductors, we first postulate a model in which the ionized impurity atoms oscillate with a natural frequency, ω_o, widely separated from the normal modes of lattice vibration in the host crystal. Since the acoustic modes pass through zero frequency this model implies that ω_o is much larger than the Debye cut-off frequency, $\omega_D = k_B\Theta/\hbar$, where Θ is the Debye temperature of the bulk material, and also smaller than the optical frequency. Therefore it is sufficient to consider the i^{th} ionized oscillating impurity atom as an isotropic harmonic oscillator with a position coordinate, $\underset{\sim}{R}_i = \underset{\sim}{R}_i(X_{i1}, X_{i2}, X_{i3})$, measured from its equilibrium position which may be taken (without loss of generality) to be the origin.

The conduction electron is then at $\underset{\sim}{r}_e = \underset{\sim}{r}_e(x_{e1}, x_{e2}, x_{e3})$ and the Hamiltonian of the system is:

$$H = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial \underset{\sim}{R}_i^2} + \tfrac{1}{2} M\omega_o^2 \underset{\sim}{R}_i^2 - \frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial \underset{\sim}{r}_e^2} - \frac{Ze^2}{\varepsilon_o |\underset{\sim}{r}_e - \underset{\sim}{R}_i|} \qquad (1\text{-}1)$$

where M and m^* are the mass of an impurity atom and the band-model effective mass of a conduction electron, ε_o is the dielectric constant

of the bulk material and Z is the excess charge of the impurity atom. We treat the last term in (1-1) as a perturbation;

$$H_{int} = - \frac{Ze^2}{\varepsilon_o |\underset{\sim}{r}_e - \underset{\sim}{R}_i|} \qquad (1\text{-}1\text{:a})$$

for which the unperturbed Hamiltonian is:

$$H^o = - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial \underset{\sim}{R}_i^2} + \tfrac{1}{2} M\omega_o^2 \underset{\sim}{R}_i^2 - \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial \underset{\sim}{r}_e^2} \qquad (1\text{-}1\text{:b})$$

and the corresponding wave function is:

$$|\underset{\sim}{n}, \underset{\sim}{k}\rangle = \chi_{\underset{\sim}{n}}(\underset{\sim}{R}_i) \cdot \psi_{\underset{\sim}{k}}(\underset{\sim}{r}_e) \qquad (1\text{-}2)$$

where the wave function of the ionized oscillating impurity atom is that of an isotropic harmonic oscillator; viz.,

$$\chi_{\underset{\sim}{n}}(\underset{\sim}{R}_i) = \prod_{j=1}^{3} \chi_{n_j}(X_{ij}) = \prod_{j=1}^{3} (\sqrt{\pi}\beta^{-1} 2^{n_j} n_j!)^{-\frac{1}{2}} H_{n_j}(\beta X_{ij}) \exp\left\{ -\tfrac{1}{2}\beta^2 X_{ij}^2 \right\} \qquad (1\text{-}2\text{:a})$$

where $\beta = \left(\frac{M\omega_o}{\hbar}\right)^{\frac{1}{2}}$ and H_{n_j} is the Hermite function, and we take the wave function for the conduction electron to be a plane wave normalized to the volume V_o of the crystal.

$$\psi_{\underset{\sim}{k}}(\underset{\sim}{r}_e) = \frac{1}{\sqrt{V_o}} e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}_e} \qquad (1\text{-}2\text{:b})$$

The energy of the unperturbed system is:

$$E^{o}_{\underset{\sim}{n}} = \hbar\omega_{o}(\underset{\sim}{n} + 3/2) + \frac{\hbar^2 k^2}{2m^*} \tag{1-3}$$

where $\underset{\sim}{n}$ is the vector with components, n_j (j=1,2,3) characterizing the state of the oscillator.

2. Scattering Matrix

For the Born approximation the matrix element for transition from a state,$(\underset{\sim}{n},\underset{\sim}{k})$, to another, $(\underset{\sim}{n}',\underset{\sim}{k}')$, is given by:

$$\langle \underset{\sim}{n}'\underset{\sim}{k}' | H_{int} | \underset{\sim}{n}\underset{\sim}{k} \rangle = - \frac{Ze^2}{\varepsilon_o V_o} \iint_{\underset{\sim}{R}_i \; \underset{\sim}{r}_e} \frac{\chi^{*}_{\underset{\sim}{n}'}(\underset{\sim}{R}_i)\chi_{\underset{\sim}{n}}(\underset{\sim}{R}_i)}{|\underset{\sim}{r}_e - \underset{\sim}{R}_i|} e^{i(\underset{\sim}{k}-\underset{\sim}{k}')\underset{\sim}{r}_e} \, d\underset{\sim}{R}_i^3 d\underset{\sim}{r}_e^3 \tag{2-1}$$

To solve (2-1), we introduce new coordinates; centre-of-mass coordinate and relative coordinate; viz.,

$$\begin{cases} \underset{\sim}{R} = \frac{1}{m}(M\underset{\sim}{R}_i + m^*\underset{\sim}{r}_e) & (2\text{-}2\text{:a}) \\ \underset{\sim}{\rho} = \underset{\sim}{r}_e - \underset{\sim}{R}_i & (2\text{-}2\text{:b}) \end{cases}$$

where $m = M + m^*$. The inverses of (2-2) are:

$$\begin{cases} \underset{\sim}{R}_i = \underset{\sim}{R} - \dfrac{m^*}{m}\,\underset{\sim}{\rho} & (2\text{-}3\text{:a}) \\ \underset{\sim}{r}_e = \underset{\sim}{R} + \dfrac{M}{m}\,\underset{\sim}{\rho} & (2\text{-}3\text{:b}) \end{cases}$$

hence (2-1) can be written in terms of the new coordinates as:

$$\langle \underset{\sim}{n'k'}|H_{int}|\underset{\sim}{nk}\rangle = -\frac{Ze^2}{\varepsilon_o V_o}\iint_{\underset{\sim}{R}\,\underset{\sim}{\rho}} \frac{\chi^*_{\underset{\sim}{n'}}(R-\frac{m^*}{m}\underset{\sim}{\rho})\,\chi_{\underset{\sim}{n}}(\underset{\sim}{R}-\frac{m^*}{m}\underset{\sim}{\rho})}{\rho}\, e^{i\underset{\sim}{K}\cdot(\underset{\sim}{R}+\frac{M}{m}\underset{\sim}{\rho})} \times |J|\, d\underset{\sim}{R}^3\, d\underset{\sim}{\rho}^3 \qquad (2\text{-}4)$$

where $|J|$ is a Jacobian:

$$|J| = \left|\frac{\partial(\underset{\sim}{r}_e,\underset{\sim}{R}_i)}{\partial(\underset{\sim}{\rho},\underset{\sim}{R})}\right| = \begin{vmatrix} \dfrac{\partial \underset{\sim}{r}_e}{\partial \underset{\sim}{\rho}} & , & \dfrac{\partial \underset{\sim}{r}_e}{\partial \underset{\sim}{R}} \\ \dfrac{\partial \underset{\sim}{R}_i}{\partial \underset{\sim}{\rho}} & , & \dfrac{\partial \underset{\sim}{R}_i}{\partial \underset{\sim}{R}} \end{vmatrix} = 1$$

and $\underset{\sim}{K} = \underset{\sim}{k} - \underset{\sim}{k'}$ is the change of the wave-vectors of a conduction electron. We now introduce the shift operator:

$$\mathbb{S}(\underset{\sim}{R}) = e^{-\underset{\sim}{\alpha}\cdot\frac{d}{d\underset{\sim}{R}}} \qquad (2\text{-}5)$$

which has the property that for any function, $F(\underset{\sim}{R})$

$$\mathbb{S}(\underset{\sim}{R})\,F(\underset{\sim}{R}) = F(\underset{\sim}{R}-\underset{\sim}{\alpha}) \qquad (2\text{-}6)$$

i.e., S operates to shift the argument of F from $\underset{\sim}{R}$ to $\underset{\sim}{R} - \underset{\sim}{\alpha}$. By use of (2-6), we find:

$$\chi^*_{\underset{\sim}{n}'}(\underset{\sim}{R}-\frac{m^*}{m}\underset{\sim}{\rho})\,\chi_{\underset{\sim}{n}}(\underset{\sim}{R}-\frac{m^*}{m}\underset{\sim}{\rho}) = e^{-\frac{m^*}{m}\underset{\sim}{\rho}\cdot\frac{d}{d\underset{\sim}{R}}}\{\chi^*_{\underset{\sim}{n}'}(\underset{\sim}{R})\chi_{\underset{\sim}{n}}(\underset{\sim}{R})\} \tag{2-7}$$

Using (2-7), the matrix element (2-4), may now be written:

$$\langle \underset{\sim}{n}'\underset{\sim}{k}'|H_{int}|\underset{\sim}{n}\underset{\sim}{k}\rangle = -\frac{Ze^2}{\varepsilon_o V_o}\int\frac{e^{i\frac{M}{m}\underset{\sim}{K}\cdot\underset{\sim}{\rho}}}{\rho}\left\{\int e^{-\frac{m^*}{m}\underset{\sim}{\rho}\frac{d}{d\underset{\sim}{R}}}\{\chi^*_{\underset{\sim}{n}'}(\underset{\sim}{R})\chi_{\underset{\sim}{n}}(\underset{\sim}{R})\}e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}}d\underset{\sim}{R}^3\right\}d\underset{\sim}{\rho}^3 \tag{2-8}$$

where the integral over $\underset{\sim}{R}$ may be evaluated by expanding the shift oprator and ignoring higher order terms, i.e.,

$$\int e^{-\frac{m^*}{m}\underset{\sim}{\rho}\frac{d}{d\underset{\sim}{R}}}\{\chi^*_{\underset{\sim}{n}'}(\underset{\sim}{R})\chi_{\underset{\sim}{n}}(\underset{\sim}{R})\}e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}}\,d\underset{\sim}{R}^3$$

$$\simeq \int(1-\frac{m^*}{m}\underset{\sim}{\rho}\cdot\frac{d}{d\underset{\sim}{R}}+\cdots\cdots)\{\chi^*_{\underset{\sim}{n}'}(\underset{\sim}{R})\chi_{\underset{\sim}{n}}(\underset{\sim}{R})\}e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}}\,d\underset{\sim}{R}^3$$

$$\simeq (1+i\frac{m^*}{m}\underset{\sim}{K}\cdot\underset{\sim}{\rho}+\cdots\cdot)\int\chi^*_{\underset{\sim}{n}'}(\underset{\sim}{R})\chi_{\underset{\sim}{n}}(\underset{\sim}{R})\,e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}}\,d\underset{\sim}{R}^3 \tag{2-9}$$

Hence substituting (2-9) into (2-8), we find:

$$\langle \underset{\sim}{n}'\underset{\sim}{k}'|H_{int}|\underset{\sim}{n}\underset{\sim}{k}\rangle \simeq -\frac{Ze^2}{\varepsilon_o V_o}\int\frac{e^{i\frac{M}{m}\underset{\sim}{K}\cdot\underset{\sim}{\rho}}}{\rho}(1+i\frac{m^*}{m}\underset{\sim}{K}\cdot\underset{\sim}{\rho})d\underset{\sim}{\rho}^3\int\chi^*_{\underset{\sim}{n}'}(\underset{\sim}{R})\chi_{\underset{\sim}{n}}(\underset{\sim}{R})e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}}d\underset{\sim}{R}^3 \tag{2-10}$$

The integral over $\underset{\sim}{\rho}$ breaks up into two parts:

$$\int_{\underset{\sim}{\rho}} \frac{e^{i\frac{M}{m}\underset{\sim}{K}\cdot\underset{\sim}{\rho}}}{\rho}\, d\underset{\sim}{\rho}^3 = \frac{4\pi}{K^2}\left(\frac{m}{M}\right)^2 \qquad (2\text{-}11\text{:a})$$

and

$$\int_{\underset{\sim}{\rho}} \frac{\underset{\sim}{K}\cdot\underset{\sim}{\rho}\, e^{i\frac{M}{m}\underset{\sim}{K}\cdot\underset{\sim}{\rho}}}{\rho}\, d\underset{\sim}{\rho}^3 = i\,\frac{8\pi}{K^2}\left(\frac{m}{M}\right)^3 \qquad (2\text{-}11\text{:b})$$

Hence (2-10) becomes, using (2-11),

$$\begin{aligned}\langle \underset{\sim}{n}'\underset{\sim}{k}'|H_{int}|\underset{\sim}{n}\underset{\sim}{k}\rangle &\simeq -\frac{4\pi Ze^2}{\varepsilon_o V_o K^2}\left(1+\frac{m^*}{M}\right)^2\left(1-2\frac{m^*}{M}\right)\int_{\underset{\sim}{R}} \chi_{\underset{\sim}{n}'}^{*}(\underset{\sim}{R})\chi_{\underset{\sim}{n}}(\underset{\sim}{R})\, e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}}\, d\underset{\sim}{R}^3 \\ &\simeq -\frac{4\pi Ze^2}{\varepsilon_o V_o K^2}\int_{\underset{\sim}{R}} \chi_{\underset{\sim}{n}'}^{*}(\underset{\sim}{R})\chi_{\underset{\sim}{n}}(\underset{\sim}{R})\, e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}}\, d\underset{\sim}{R}^3 \qquad (2\text{-}12)\end{aligned}$$

since $\frac{m^*}{M} << 1$, where $\underset{\sim}{K} = \underset{\sim}{k}-\underset{\sim}{k}'$ and $\chi_{\underset{\sim}{n}}(\underset{\sim}{R})$ is given by (1-2:a).

The first factor in (2-12) leads to the ordinary Coulomb scattering from a stationary nucleus but the integral modifies the matrix element through the oscillations of the impurity centre. We note that when statistical averages are taken, both $\underset{\sim}{n}$ and $\underset{\sim}{K}$ will depend on the temperature and hence the integral indicates the possibility of a modification in the temperature dependence for ionized impurity

scattering from that given by the Conwell-Weisskopf formula.

2-1 Scattering from the Zero-point Oscillations

It is instructive to examine the effect of the zero-point oscillation of the ionized impurity atom; at the absolute zero temperature, $T = 0^{\circ}K$, the ionized oscillating impurity atom is in the ground state, i.e., $\underset{\sim}{n}' = \underset{\sim}{n} = 0$. In this case the integral in (2-12) may be written:

$$\prod_{j=1}^{3} I_o^j = \prod_{j=1}^{3} \int_{X_j} \chi_o^*(X_j)\chi_o(x_j)\, e^{iK_jX_j}\, dX_j \qquad (2\text{-}13)$$

where the ground state wave function is:

$$\chi_o(X_j) = (\sqrt{\pi}\beta^{-1})^{-\frac{1}{2}} \exp(-\tfrac{1}{2}\beta^2 X_j^2), \qquad j = 1,2,3. \qquad (2\text{-}14)$$

Hence:

$$I_o^j = \int_{-\infty}^{\infty} \chi_o^*(X_j)\chi_o(X_j)\, e^{iK_j\cdot X_j}\, dX_j = (\tfrac{\beta}{\sqrt{\pi}}) e^{-\frac{K_j^2}{4\beta^2}} \int_{-\infty}^{\infty} e^{-\beta^2(X_j - \frac{iK}{2\beta^2})^2}\, dX_j$$

$$= e^{-K_j^2/4\beta^2}$$

so that (2-13) becomes:

$$\prod_{j=1}^{3} I_o^j = \prod_{j=1}^{3} e^{-K_j^2/4\beta^2} = \exp\left\{-\sum_{j=1}^{3} K_j^2/4\beta^2\right\} = \exp\left\{-K^2/4\beta^2\right\}$$

The matrix element for the ground state is thus:

$$\langle 0,\underset{\sim}{k}'|H_{int}|0,\underset{\sim}{k}\rangle = -\frac{4\pi Ze^2}{\varepsilon_o V_o K^2}\, e^{-K^2/4\beta^2} \qquad (2\text{-}15)$$

where $\underset{\sim}{K} = \underset{\sim}{k} - \underset{\sim}{k}'$ and $\beta = \left(\frac{M\omega_o}{\hbar}\right)^{\frac{1}{2}}$

We note that (2-15) becomes the matrix element for pure Coulomb scattering from a stationary impurity nucleus only when $\beta \to \infty$; i.e., $M \to \infty$ or $\omega_o \to \infty$. The exponential factor in (2-15) can be written as :

$$\exp\left\{-\frac{(\underset{\sim}{k} - \underset{\sim}{k}')^2}{4\beta^2}\right\} = \exp\left\{-\frac{3}{4}\left(\frac{\hbar^2(\underset{\sim}{k} - \underset{\sim}{k}')^2}{2M}\right)/\left(\frac{3\hbar\omega_o}{2}\right)\right\}$$

$$= \exp\left\{-\frac{3}{4}\left(\frac{\text{Recoil energy of the impurity nucleus}}{\text{Zero-point energy of the impurity nucleus}}\right)\right\} \qquad (2\text{-}16)$$

This shows that when the recoil energy of the impurity nucleus is very small compared to the zero-point energy of the oscillating impurity, the Conwell - Weisskopf result is exactly recovered. For larger recoil, the matrix element may be reduced and may lead to an enhanced mobility of the conduction electrons.

2-2 Elastic Scattering at Finite Temperatures

When $T > 0^{\circ}K$, we must consider the integral in (2-12) for an arbitrary excitation; i.e., $\underset{\sim}{n}$ and $\underset{\sim}{n}'$ are not zero. The case, $\underset{\sim}{n} = \underset{\sim}{n}'$,

leads to the elastic scattering, but $\underset{\sim}{n} \neq \underset{\sim}{n}'$ involves the emission or absorption of one or more phonons and leads to inelastic scattering. Here we consider only the elastic scattering case, i.e., $\underset{\sim}{n} = \underset{\sim}{n}'$.

For finite $\underset{\sim}{n}$; i.e., $n_j \neq 0$ (j = 1,2,3), we must calculate the integral:

$$\mathbf{I}^{j}_{n_j} = \int_{-\infty}^{\infty} \chi^{*}_{n_j}(X_j)\, \chi_{n_j}(X_j)\, e^{iK_j X_j}\, dX_j \tag{2-17}$$

where $\chi_{n_j}(X_j)$, the normalized simple harmonic oscillator wave function, is given by:

$$\chi_{n_j}(X_j) = (\sqrt{\pi}\beta^{-1} 2^{n_j} n_j!)^{-\frac{1}{2}}\, H_{n_j}(\beta X_j)\, e^{-\frac{1}{2}\beta^2 X_j^2} \tag{2-18}$$

Letting $\eta = \beta X_j$, there results:

$$\mathbf{I}^{j}_{n_j} = (\sqrt{\pi} 2^{n_j} n_j!)^{-1} \int_{-\infty}^{\infty} e^{-\eta^2}\, e^{i(K_j/\beta)\eta}\, H^{2}_{n_j}(\eta)\, d\eta \tag{2-19}$$

To evaluate (2-19), we introduce the generating function and for the Hermite polynomials (e.g.,see Margenau and Murphy (1956)):

$$e^{2tx - t^2} = \sum_{\lambda=0}^{\infty} \frac{t^{\lambda}}{\lambda!} H_{\lambda}(x) \tag{2-20}$$

In our case, $t \equiv iK_j/2\beta$ and $x \equiv \eta$, so that:

$$e^{iK_j\eta/\beta} \equiv e^{-K_j^2/4\beta^2} \sum_{\lambda=0}^{\infty} \frac{i^\lambda}{\lambda!}\left(\frac{K_j}{2\beta}\right)^\lambda H_\lambda(\eta) \qquad (2\text{-}21)$$

Substituting (2-21) into (2-19), the integral (2-17) is:

$$I^j_{n_j} = (\sqrt{\pi}\, 2^{n_j}\, n_j!)^{-1}\, e^{-K_j^2/4\beta^2} \sum_{\lambda=0}^{\infty} \frac{i^\lambda}{\lambda!}\left(\frac{K_j}{2\beta}\right)^\lambda \int_{-\infty}^{\infty} e^{-\eta^2} H_\lambda(\eta) H_{n_j}^2(\eta)\, d\eta \qquad (2\text{-}22)$$

Since $H_{n_j}^2(\eta)$ is an even function of η, in order to calculate the non-zero solution, λ must be an even integer. Letting $\lambda = 2p$ ($p = 0,1,2,\cdots\cdots\cdots$), (2-22) becomes:

$$I^j_{n_j} = (\sqrt{\pi}\, 2^{n_j}\, n_j!)^{-1}\, e^{-K_j^2/4\beta^2} \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p)!}\left(\frac{K_j^2}{4\beta^2}\right)^p \mathbf{I}_{p,n_j} \qquad (2\text{-}23)$$

where $\mathbf{I}_{p,n_j}$ is:

$$\mathbf{I}_{p,n_j} \equiv \int_{-\infty}^{\infty} e^{-\eta^2} H_{2p}(\eta) H_{n_j}^2(\eta)\, d\eta \qquad j = 1,2,3. \qquad (2\text{-}24)$$

To evaluate the integral, (2-24), we now make use of the identity:

$$e^{-\eta^2} H_n(\eta) \equiv -\frac{d}{d\eta}\left(e^{-\eta^2} H_{n-1}(\eta)\right) \qquad (2\text{-}25)$$

so that:

$$\mathbb{I}_{p,n} = -\int_{-\infty}^{\infty} H_{2p}(\eta)H_n(\eta)\frac{d}{d\eta}(e^{-\eta^2}H_{n-1}(\eta))\,d\eta \qquad (2\text{-}26)$$

and by partial integration, (2-26) becomes:

$$\mathbb{I}_{p,n} = \int_{-\infty}^{\infty} e^{-\eta^2}H_{n-1}(\eta)\frac{d}{d\eta}(H_{2p}(\eta)H_n(\eta))\,d\eta$$

Again by use of (2-25) and partial integration,

$$\mathbb{I}_{p,n} = \int_{-\infty}^{\infty} e^{-\eta^2}H_{n-2}(\eta)\frac{d^2}{d\eta^2}(H_{2p}(\eta)H_n(\eta))\,d\eta$$

so that repeating in this manner, we finally obtain the result:

$$\mathbb{I}_{p,n} = \int_{-\infty}^{\infty} e^{-\eta^2}H_o(\eta)\frac{d^n}{d\eta^n}(H_{2p}(\eta)H_n(\eta))\,d\eta .$$

But since $H_o(\eta) = 1$, we have the final expression of $\mathbb{I}_{p,n}$

$$\mathbb{I}_{p,n} = \int_{-\infty}^{\infty} e^{-\eta^2}\frac{d^n}{d\eta^n}(H_{2p}(\eta)H_n(\eta))\,d\eta \qquad (2\text{-}27)$$

It is now easy to evaluate (2-27) for small values of n;

(i) n = 0

$$\mathbb{I}_{p,n} = \int_{-\infty}^{\infty} e^{-\eta^2}H_{2p}(\eta)H_o(\eta)\,d\eta = \sqrt{\pi}\,\delta_{p,0}$$

where use has been made of the orthogonal result; viz.,

$$\int_{-\infty}^{\infty} e^{-\eta^2} H_m(\eta) H_n(\eta) d\eta = \sqrt{\pi}\, 2^n\, n!\, \delta_{m,n} \tag{2-28}$$

(ii) n = 1

$$I_{p,1} = \int_{-\infty}^{\infty} e^{-\eta^2} \frac{d}{d\eta} \left\{ H_{2p}(\eta) H_1(\eta) \right\} d\eta = \int_{-\infty}^{\infty} e^{-\eta^2} \left\{ H_{2p}(\eta) H_1'(\eta) + H_{2p}'(\eta) H_1(\eta) \right\} d\eta$$

By use of the recurrence formula, viz.,

$$H_n'(\eta) = 2n H_{n-1}(\eta) \tag{2-29}$$

and of (2-28), we obtain:

$$I_{p,1} = 2 \int_{-\infty}^{\infty} e^{-\eta^2} H_{2p}(\eta) H_o(\eta) d\eta + 4p \int_{-\infty}^{\infty} e^{-\eta^2} H_{2p-1}(\eta) H_1(\eta) d\eta$$

$$= 2\sqrt{\pi}\, \delta_{p,0} + 8\sqrt{\pi} p\, \delta_{p,1}$$

(iii) n = 2

$$I_{p,2} = \int_{-\infty}^{\infty} e^{-\eta^2} \frac{d^2}{d\eta^2} \left\{ H_{2p}(\eta) H_2(\eta) \right\} d\eta$$

$$= \int_{-\infty}^{\infty} e^{-\eta^2} \frac{d}{d\eta} \left\{ H_{2p}(\eta) H_2'(\eta) + H_{2p}'(\eta) H_2(\eta) \right\} d\eta$$

$$= \int_{-\infty}^{\infty} e^{-\eta^2} \frac{d}{d\eta} \left\{ 4H_{2p} H_1 + 4pH_{2p-1} H_2 \right\} d\eta \qquad \text{(By use of (2-29))}$$

$$= \int_{-\infty}^{\infty} e^{-\eta^2} \left\{ 4H_{2p} H_1' + 4H_{2p}' H_1 + 4pH_{2p-1} H_2' + 4pH_{2p-1}' H_2 \right\} d\eta$$

$$= \int_{-\infty}^{\infty} e^{-\eta^2} \left\{ 8H_{2p} H_o + 16pH_{2p-1} H_1 + 16pH_{2p-1} H_1 + 8p(2p-1) H_{2p-2} H_2 \right\} d\eta$$

(By use of (2-29))

$$= 8\sqrt{\pi}\, \delta_{p,0} + 64\sqrt{\pi}\, p\delta_{p,1} + 64\sqrt{\pi} p(2p-1)\, \delta_{p,2}$$

(By use of (2-28))

(iv) n = 3

$$I_{p,3} = 48\sqrt{\pi}\, \delta_{p,0} + 576\sqrt{\pi}\, \delta_{p,1} + 192\sqrt{\pi}\, p(2p-1)\, \delta_{p,3/2}$$

$$+ 384\sqrt{\pi}\, p(2p-1)\, \delta_{p,2} + 1536\sqrt{\pi}\, p(p-1)(2p-1)\, \delta_{p,3}$$

(v) $n = 4$

$$I_{p,4} = 384\sqrt{\pi}\,\delta_{p,0} + 1536\sqrt{\pi}\,(3p+1)\,\delta_{p,1} + 3072\sqrt{\pi}\,(2p-1)(5p+1)\,\delta_{p,2}$$

$$+49152\sqrt{\pi}\,p(p-1)(2p-1)\,\delta_{p,3} + 24576\sqrt{\pi}\,p(p-1)(2p-1)(2p-3)\,\delta_{p,4}$$

From these results we deduce that:

$$I^{j}_{n_j} = P^{j}_{n_j}\left(\frac{K_j^2}{\beta^2}\right) e^{-K_j^2/4\beta^2} \qquad (2\text{-}30)$$

where $P^{j}_{n_j}$ is a polynomial of degree n_j with argument, K_j^2/β^2, and may be expressed as:

$$P^{j}_{n_j}\left(\frac{K_j^2}{\beta^2}\right) \to \begin{cases} 1 \text{ for } K_j << \beta & (2\text{-}31:a) \\ \sum_{n_j=0}^{n_j} \dfrac{(-1)^{n_j}}{2^{n_j}\, n_j!}\left(\dfrac{K_j^2}{\beta^2}\right)^{n_j} \quad \text{for } K_j >> \beta & (2\text{-}31:b) \end{cases}$$

$(j = 1,2,3)$

By use of (2-30), the matrix element, (2-12), for scattering due to the ionized oscillating impurity with a localized frequency widely separated from the normal modes of the host atoms is:

$$\langle \underset{\sim}{n}\underset{\sim}{k}' | H_{int} | \underset{\sim}{n}\underset{\sim}{k} \rangle = -\frac{4\pi Ze^2}{\varepsilon_o V_o K^2} \prod_{j=1}^{3} P^{j}_{n_j}\left(\frac{K_j^2}{\beta^2}\right) e^{-K_j^2/4\beta^2} \qquad (2\text{-}32)$$

where the polynomial, $P^{j}_{n_j}$, is given by (2-31:a,b) and $K_j^2 = |k_j - k'_j|^2$. We note here that the factor,

$$\prod_{j=1}^{3} P^{j}_{n_j} \cdot e^{-K_j^2/4\beta^2}$$

is due to the impurity oscillation and that if $\beta \to \infty$, (2-32) becomes the ordinary pure "Coulomb" scattering matrix element for electron scattering from a fixed scattering centre, and leads to the Conwell-Weisskopf formula.

3. Mean-Free-Time and Relaxation Time for Momentum Transfer

3-1 Mean-Free-Time

The matrix element for the elastic scattering of a conduction electron from a state, $\underset{\sim}{k}$, to another, $\underset{\sim}{k}'$, by interaction with a localized oscillating ionized impurity atom in the state, $\underset{\sim}{n}$, is given by (2-32); viz.,

$$\langle \underset{\sim}{n}\underset{\sim}{k}' | H_{int} | \underset{\sim}{n}\underset{\sim}{k} \rangle = - \frac{4\pi Ze^2}{\varepsilon_o V_o K^2} \prod_{j=1}^{3} P^{j}_{n_j}\left(\frac{K_j^2}{\beta^2} \right) \cdot e^{-K_j^2/4\beta^2} \qquad (3\text{-}1)$$

where $\underset{\sim}{K} = \underset{\sim}{k} - \underset{\sim}{k}'$, $\beta = (M\omega_o/\hbar)^{\frac{1}{2}}$ and $P^{j}_{n_j}$ is given by (2-31). We may now calculate the mean-free-time of a conduction electron by use of the microscopic transition probability per second based on Fermi's Golden rule, viz.,

$$P_{\underset{\sim}{n}\underset{\sim}{k}\rightarrow\underset{\sim}{n}\underset{\sim}{k}'} = \frac{2\pi}{\hbar} |\langle \underset{\sim}{n}\underset{\sim}{k}' | H_{int} | \underset{\sim}{n}\underset{\sim}{k} \rangle|^2 \, \delta(E_{\underset{\sim}{n}\underset{\sim}{k}'} - E_{\underset{\sim}{n}\underset{\sim}{k}}) \qquad (3\text{-}2)$$

where the initial and the final energies of the system are:

$$E_{\underset{\sim}{n},\underset{\sim}{k}} = \hbar\omega_o(\underset{\sim}{n} + 3/2) + \frac{\hbar^2 k^2}{2m^*} \qquad (3\text{-}3\text{:a})$$

$$E_{\underset{\sim}{n},\underset{\sim}{k}'} = \hbar\omega_o(\underset{\sim}{n} + 3/2) + \frac{\hbar^2 k'^2}{2m^*} \qquad (3\text{-}3\text{:b})$$

Since for elastic processes the oscillata states do not change, the δ-function in (3-2) ensures the energy conservation of the system . This implies :

$$k = k' \qquad (3\text{-}4)$$

To find the mean-free-time of the conduction electrons, we must appeal to the electronic distribution function, $f(\underset{\sim}{k},t)$, such that:

$$\frac{V_o}{8\pi^3} f(\underset{\sim}{k},t) \, d\underset{\sim}{k}^3 \qquad (3\text{-}5)$$

is the number of conduction electrons with wave numbers between $\underset{\sim}{k}$ and $\underset{\sim}{k}+d\underset{\sim}{k}$. Here $f(\underset{\sim}{k},t)$ is a dimensionless quantity. The rate of change of $f(\underset{\sim}{k})$ due to scattering of electrons from a state, $\underset{\sim}{k}$, to another state, $\underset{\sim}{k}'$, by the interaction with all the localized oscillating

ionized impurity atoms in various states, $\underset{\sim}{n}$, may be given by:

$$\left.\frac{\partial f(\underset{\sim}{k})}{\partial t}\right]_{\text{Loss}} = -\sum_{\underset{\sim}{n}}\sum_{\underset{\sim}{k}'} F_{\underset{\sim}{n}} P_{\underset{\sim}{n}\underset{\sim}{k}\to\underset{\sim}{n}\underset{\sim}{k}'} f(\underset{\sim}{k})\left\{1-f(\underset{\sim}{k}')\right\} \tag{3-6}$$

where $\sum_{\underset{\sim}{n}} \equiv \sum_{n_1}\sum_{n_2}\sum_{n_3}$ and $F_{\underset{\sim}{n}}$ is the number of localized oscillating ionized impurity atoms in a state, $\underset{\sim}{n}$.

Similarly, the rate of change of $f(\underset{\sim}{k})$ due to the inverse scattering processes of conduction electrons from a state, $\underset{\sim}{k}'$, to another, $\underset{\sim}{k}$, by the interaction with the localized oscillating ionized impurity atoms may be given by:

$$\left.\frac{\partial f(\underset{\sim}{k})}{\partial t}\right]_{\text{gain}} = \sum_{\underset{\sim}{n}}\sum_{\underset{\sim}{k}'} F_{\underset{\sim}{n}} P_{\underset{\sim}{n}\underset{\sim}{k}'\to\underset{\sim}{n}\underset{\sim}{k}} f(\underset{\sim}{k}')\left\{1-f(\underset{\sim}{k})\right\} \tag{3-7}$$

We note that, in (3-6) and (3-7), we have introduced the Fermi statistics to the electrons and employed the probabilities of unoccupancy of electron; $1-f(\underset{\sim}{k}')$ and $1-f(\underset{\sim}{k})$, which make sure the electrons to be scattered into either the $\underset{\sim}{k}'$- or $\underset{\sim}{k}$- states. We assume that the impurity atoms are in good thermal contact with the host atoms, so that at temperature, T, $F_{\underset{\sim}{n}}$ is determined by its equilibrium value; viz.,

$$F_{\underset{\sim}{n}} = \frac{N_D^{(+)}}{\sigma}\exp\left\{-(\underset{\sim}{n}+3/2)\,\hbar\omega_o/k_BT\right\} \tag{3-8}$$

where $N_D^{(+)}$ is the total number of the localized oscillating ionized impurity atoms and σ is the partition function of a three dimensional isotropic oscillator.

By adding (3-6) and (3-7) we have the net rate of change of $f(\underset{\sim}{k},t)$:

$$\left.\frac{\partial f(\underset{\sim}{k})}{\partial t}\right]_{net} = \left.\frac{\partial f(\underset{\sim}{k})}{\partial t}\right]_{gain} + \left.\frac{\partial f(\underset{\sim}{k})}{\partial t}\right]_{loss}$$

$$= \sum_{\underset{\sim}{n}} \sum_{\underset{\sim}{k}'} \mathbf{F}_{\underset{\sim}{n}} P_{\underset{\sim}{n}\underset{\sim}{k}\to\underset{\sim}{n}\underset{\sim}{k}'} \left\{ f(\underset{\sim}{k}') - f(\underset{\sim}{k}) \right\} \qquad (3\text{-}9)$$

where we have used the property of microreversibility, i.e.,

$$P_{\underset{\sim}{n}\underset{\sim}{k}\to\underset{\sim}{n}\underset{\sim}{k}'} = P_{\underset{\sim}{n}\underset{\sim}{k}'\to\underset{\sim}{n}\underset{\sim}{k}}$$

We may write (3-9) as follows:

$$\frac{\partial f(\underset{\sim}{k})}{\partial t} = A(\underset{\sim}{k}) - B(\underset{\sim}{k}) \cdot f(\underset{\sim}{k}) \qquad (3\text{-}10)$$

where

$$\begin{cases} A(\underset{\sim}{k}) = \sum_{\underset{\sim}{n}} \sum_{\underset{\sim}{k}'} \mathbf{F}_{\underset{\sim}{n}} P_{\underset{\sim}{n}\underset{\sim}{k}\to\underset{\sim}{n}\underset{\sim}{k}'} f(\underset{\sim}{k}') & (3\text{-}10\text{:a}) \\ B(\underset{\sim}{k}) = \sum_{\underset{\sim}{n}} \sum_{\underset{\sim}{k}'} \mathbf{F}_{\underset{\sim}{n}} P_{\underset{\sim}{n}\underset{\sim}{k}\to\underset{\sim}{n}\underset{\sim}{k}'} & (3\text{-}10\text{:b}) \end{cases}$$

If we assume that $f(\underset{\sim}{k})$ is not too far from its equilibrium value, we may regard $A(\underset{\sim}{k})$ as a slowly varying function of time and (3-10) may be then integrated to give:

$$f(\underset{\sim}{k}) = \frac{A(\underset{\sim}{k})}{B(\underset{\sim}{k})} + \zeta e^{-B(\underset{\sim}{k})t} \tag{3-11}$$

As $t \to \infty$, the distribution function, $f(\underset{\sim}{k})$, must attain its equilibrium value; viz.,

$$f^{o}(\underset{\sim}{k}) = \left\{\exp(E(\underset{\sim}{k}) - \mu)/k_B T + 1\right\}^{-1} \tag{3-12}$$

so that $A(\underset{\sim}{k})/B(\underset{\sim}{k}) = f^{o}(\underset{\sim}{k})$ and we obtain:

$$f(\underset{\sim}{k}) = f^{o}(\underset{\sim}{k}) + \zeta e^{-B(\underset{\sim}{k})t} \tag{3-13}$$

Clearly we see that B(k) acts as a reciprocal relaxation time for the distribution function to approach equilibrium. It is, in fact, the mean-free-time of a conduction electron, viz.,

$$\frac{1}{\tau^{(f)}_{\underset{\sim}{k}}} = \sum_{\underset{\sim}{n}} \sum_{\underset{\sim}{k}'} F_{\underset{\sim}{n}} P_{\underset{\sim}{n}\underset{\sim}{k} \to \underset{\sim}{n}\underset{\sim}{k}'} \tag{3-14}$$

From (3-10, 11, 13, 14), we have:

$$\frac{\partial f(\underset{\sim}{k})}{\partial t} = -B(\underset{\sim}{k}) \zeta e^{-B(\underset{\sim}{k})t}$$

$$= -B(\underset{\sim}{k}) \{ f(\underset{\sim}{k}) - f^{\circ}(\underset{\sim}{k}) \}$$

$$= - \frac{f(\underset{\sim}{k}) - f^{\circ}(\underset{\sim}{k})}{\tau^{(f)}_{\underset{\sim}{k}}} \qquad (3\text{-}15)$$

and (3-15) is the usual form of the collision term employed in the Boltzmann's equation. Using (3-1),(3-2), (3-3:a,b) and (3-8) in (3-14) we may obtain the explicit form of the mean-free-time of a conduction electron. But of greater interest for mobility calculation is the relaxation time for momentum transfer considered in detail in the next section.

3-2 Relaxation Time for Momentum Transfer

A conduction electron being scattered from a state, $\underset{\sim}{k}$, to another state, $\underset{\sim}{k}'$, by a localized oscillating ionized impurity suffers a momentum loss:

$$\Delta \underset{\sim}{p}(\underset{\sim}{k}) = \hbar \, (\underset{\sim}{k} - \underset{\sim}{k}') \qquad (3\text{-}16)$$

Therefore, the total rate, at which linear momentum is being transfered from all the electrons with wave numbers between $\underset{\sim}{k}$ and $\underset{\sim}{k} + d\underset{\sim}{k}$ to all of the localized oscillating ionized impurity centres, is:

$$\left. \frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t} \right]_{loss} = - \sum_{\underset{\sim}{n}} \sum_{\underset{\sim}{k}'} \hbar(\underset{\sim}{k}-\underset{\sim}{k}') \underset{\sim}{F}_{\underset{\sim}{n}} \, P_{\underset{\sim}{n}\underset{\sim}{k} \rightarrow \underset{\sim}{n}\underset{\sim}{k}'} \, f(\underset{\sim}{k}) \{ 1-f(\underset{\sim}{k}') \}$$

(3-17)

Similarly, the total rate, at which linear momentum is being gained by all the conduction electrons with wave numbers between $\underset{\sim}{k}$ and $\underset{\sim}{k}+d\underset{\sim}{k}$ through interaction with all the impurities, is:

$$\left.\frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t}\right]_{gain} = \sum_{\underset{\sim}{n}} \sum_{\underset{\sim}{k}'} \hbar(\underset{\sim}{k}-\underset{\sim}{k}') \mathbf{F}_{\underset{\sim}{n}} P_{\underset{\sim}{n}\underset{\sim}{k}'\rightarrow\underset{\sim}{n}\underset{\sim}{k}} f(\underset{\sim}{k}') \left\{1-f(\underset{\sim}{k})\right\} \qquad (3\text{-}18)$$

Consequently the net rate, at which linear momentum is being gained by all the conduction electrons with wave numbers between $\underset{\sim}{k}$ and $\underset{\sim}{k}+d\underset{\sim}{k}$ through interaction with all the impurities, is:

$$\left.\frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t}\right]_{net} = \left.\frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t}\right]_{gain} + \left.\frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t}\right]_{loss}$$

$$= \sum_{\underset{\sim}{n}} \sum_{\underset{\sim}{k}'} \hbar(\underset{\sim}{k}-\underset{\sim}{k}') \mathbf{F}_{\underset{\sim}{n}} P_{\underset{\sim}{n}\underset{\sim}{k}\rightarrow\underset{\sim}{n}\underset{\sim}{k}'} \left\{ f(\underset{\sim}{k}') - f(\underset{\sim}{k})\right\} \qquad (3\text{-}19)$$

where use has been made of the property of microreversibility;

$$P_{\underset{\sim}{n}\underset{\sim}{k}\rightarrow\underset{\sim}{n}\underset{\sim}{k}'} = P_{\underset{\sim}{n}\underset{\sim}{k}'\rightarrow\underset{\sim}{n}\underset{\sim}{k}}$$

Since the total linear momentum of all the conduction electrons with wave numbers between $\underset{\sim}{k}$ and $\underset{\sim}{k}+d\underset{\sim}{k}$ is:

$$\underset{\sim}{M}(\underset{\sim}{k}) = \hbar\underset{\sim}{k}\, f(\underset{\sim}{k}) \qquad (3\text{-}20)$$

(3-19) becomes:

$$\hbar\underset{\sim}{k}\,\frac{\partial f(\underset{\sim}{k})}{\partial t} = \sum_{n}\sum_{\underset{\sim}{k}'} \hbar(\underset{\sim}{k}-\underset{\sim}{k}')\,\mathbf{F}_{n}\,P_{n\underset{\sim}{k}\to n\underset{\sim}{k}'}\,\{f(\underset{\sim}{k}') - f(\underset{\sim}{k})\}$$

or

$$\frac{\partial f(\underset{\sim}{k})}{\partial t} = A(\underset{\sim}{k}) - B(\underset{\sim}{k})\cdot f(\underset{\sim}{k}) \qquad (3\text{-}21)$$

where:

$$\left\{\begin{array}{l} A(\underset{\sim}{k}) = \sum_{n}\sum_{\underset{\sim}{k}'} \left\{1 - \frac{\underset{\sim}{k}'\cdot\underset{\sim}{k}}{k^2}\right\}\mathbf{F}_{n}\,P_{n\underset{\sim}{k}\to n\underset{\sim}{k}'}\,f(\underset{\sim}{k}') \qquad (3\text{-}21\text{:a}) \\ B(\underset{\sim}{k}) = \sum_{n}\sum_{\underset{\sim}{k}'} \left\{1 - \frac{\underset{\sim}{k}'\cdot\underset{\sim}{k}}{k^2}\right\}\mathbf{F}_{n}\,P_{n\underset{\sim}{k}\to n\underset{\sim}{k}'} \qquad (3\text{-}21\text{:b}) \end{array}\right.$$

Clearly $B(\underset{\sim}{k})$ acts like a reciprocal relaxation Time for Momentum transfer to the localized oscillating ionized impurity centres; i.e.,

$$\frac{1}{\tau_i(\underset{\sim}{k})} = \sum_{n}\sum_{\underset{\sim}{k}'}\left\{1 - \frac{\underset{\sim}{k}\cdot\underset{\sim}{k}'}{k^2}\right\}\mathbf{F}_{n}\,P_{n\underset{\sim}{k}\to n\underset{\sim}{k}'} \qquad (3\text{-}22)$$

where $\mathbf{F}_{n}$ and $P_{n\underset{\sim}{k}\to n\underset{\sim}{k}'}$ are given by (3-8) and by (3-2) with (3-1) and with (3-3:a,b), respectively. Employing (3-1) and (3-2) becomes:

$$\frac{1}{\tau_i} = \frac{2\pi}{\hbar}\left(\frac{4\pi Ze^2}{\epsilon_o V_o}\right)^2 \sum_{n}\sum_{\underset{\sim}{k}'}\mathbf{F}_{n}\left\{\prod_{j=1}^{3} P^{j}_{n_j}\left(\frac{K_j^2}{\beta^2}\right)\right\}^2 \frac{1 - \frac{\underset{\sim}{k}\cdot\underset{\sim}{k}'}{k^2}}{(\underset{\sim}{k}-\underset{\sim}{k}')^4}$$

$$\times\, e^{-(\underset{\sim}{k}-\underset{\sim}{k}')^2/2\beta^2}\,\delta(E_{n\underset{\sim}{k}'} - E_{n\underset{\sim}{k}}) \qquad (3\text{-}23)$$

It is now convenient to replace the summation over the final state, $\underset{\sim}{k}'$, by the integral as a usual manner; viz.,

$$\sum_{\underset{\sim}{k}'} (\cdots\cdots\cdots) = \frac{V_o}{8\pi^3} \int_{\underset{\sim}{k}'} (\cdots\cdots\cdots)\, d\underset{\sim}{k}'^3 \tag{3-24}$$

so that using (3-24), (3-23) becomes:

$$\frac{1}{\tau_i} = \frac{4\, Z^2 e^4}{\hbar \varepsilon_o^2 V_o} \sum_{\underset{\sim}{n}} \int F_{\underset{\sim}{n}} \left\{ \prod_{j=1}^{3} P_{n_j}^{j} \left(\frac{K_j^2}{\beta^2} \right) \right\}^2 \frac{1 - \frac{\underset{\sim}{k} \cdot \underset{\sim}{k}'}{k^2}}{(\underset{\sim}{k} - \underset{\sim}{k}')^4}$$
$$\times\, e^{-(\underset{\sim}{k}-\underset{\sim}{k}')^2/2\beta^2}\, \delta(E_{\underset{\sim}{n}\underset{\sim}{k}'} - E_{\underset{\sim}{n}\underset{\sim}{k}})\, d\underset{\sim}{k}'^3 \tag{3-25}$$

where $\sum_{\underset{\sim}{n}} = \sum_{n_1} \sum_{n_2} \sum_{n_3}$

To evaluate (3-25), we establish $\underset{\sim}{k}$ along the x_3-axis in the Cartesian coordinates, and let $\underset{\sim}{k}'$ make angles, θ and ϕ, in the polar coordinates.

From (3-3:a,b) we have:

$$E_{\underset{\sim}{n}\underset{\sim}{k}'} - E_{\underset{\sim}{n}\underset{\sim}{k}} = \frac{\hbar^2}{2m^*} (\underset{\sim}{k}'^2 - \underset{\sim}{k}^2)$$

from which:

$$k'^2 dk' = \frac{m^* k'}{\hbar^2}\, d(E_{\underset{\sim}{n}\underset{\sim}{k}'} - E_{\underset{\sim}{n}\underset{\sim}{k}}) \tag{3-26}$$

so that (3-25) becomes:

$$\frac{1}{\tau_i} = \frac{4\,Z^2e^4}{\hbar\varepsilon_o{}^2V_o} \sum_{\underset{\sim}{n}} \iiint F_{\underset{\sim}{n}} \left\{ \prod_{j=1}^{3} P_{n_j}^{j}\left(\frac{K_j^2}{\beta^2}\right) \right\}^2 \frac{1 - \frac{k'}{k}\cos\theta}{(k^2+k'^2-2kk'\cos\theta)^2}$$

$$\times \left\{ \exp\left\{ -(k^2+k'^2-2kk'\cos\theta)/2\beta^2 \right\} \right\} \delta(E_{\underset{\sim}{n}k'} - E_{\underset{\sim}{n}k}) \frac{m^* k'}{\hbar^2}$$

$$\times\, d(E_{\underset{\sim}{n}k'} - E_{\underset{\sim}{n}k}) \sin\theta d\theta d\phi \qquad (3\text{-}27)$$

Noting that the integral over the energy contributes only when $k' = k$, we have:

$$\frac{1}{\tau_i} = \frac{2\pi Z^2 e^4 m^*}{\hbar^3 \varepsilon_o{}^2 V_o k^3} \sum_{\underset{\sim}{n}} \int F_{\underset{\sim}{n}} \left\{ \prod_{j=1}^{3} P_{n_j}^{j}\left(\frac{K_j^2}{\beta^2}\right) \right\}^2_{k'=k} \frac{\sin\theta}{1-\cos\theta}$$

$$\times \exp\left\{ -(1 - \cos\theta)\frac{k^2}{\beta^2} \right\} d\theta \qquad (3\text{-}28)$$

We note here that the above integral diverges at $\theta=0$. This is the usual "Coulomb cross section divergency" which may be eliminated by introducing the fact that small angle scattering has to do with electrons whose distance of closest approach to the scattering centre is very large, or by introducing the screening factor of electrons which screen the scattering centre and cut off the long range effect of Coulomb field at a certain distance. There is thus a limit to the smallness of the scattering angle possible since for great enough distances the electron will see not only the scattering centre in question

but also the next-nearest-neighbour scattering centre. The lower limit on θ in the integral in (3-28) is thus given by the scattering of electrons whose impact parameters are approximately half the mean distance, L, say, between nearest neighbour scattering centres. We now note that the greatest contribution to the integral in (3-28) comes from small angle scattering. Hence we may take the polynomial being approximately unity. We may then perform the sum over $\underset{\sim}{n}$ easily to give the total number of impurity atoms; i.e.,

$$\sum_{\underset{\sim}{n}} \mathbf{F}_{\underset{\sim}{n}} = N_D^{(+)} = n_D^{(+)} V_o$$

where $n_D^{(+)}$ is the impurity concentration given in terms of impurity spacing, L; $n_D^{(+)} = L^{-3}$. We, therefore, have (3-28) as:

$$\frac{1}{\tau_i} = \frac{2\pi Z^2 e^4 m^* n_D^{(+)}}{\varepsilon_o^2 \hbar^3 k^3} \int_{\theta=\theta_{min}}^{\pi} \frac{\sin\theta}{1 - \cos\theta} e^{-\frac{k^2}{\beta^2}(1 - \cos\theta)} \, d\theta \qquad (3\text{-}29)$$

We note that (3-29) leads to the Conwell-Weisskopf result if β goes to ∞.

3-3 Determination of Small Scattering Angle

Before proceeding the calculation of (3-29), we must determine, θ_{min}, the small scattering angle. From the dynamics of collisions (Goldstein, (1950)), the relative velocity of the electron, v, its impact parameter,

b, and the scattering angle, θ, are connected by the Rutherford scattering formula; viz.,

$$\tan \frac{\theta}{2} = \frac{Ze^2}{\varepsilon_o b} \Big/ \frac{m^* v^2}{2} \tag{3-30}$$

As mentioned in the previous section, the limitation on impact parameter is equivalent to the limitation on θ. For the largest impact parameter, $b = L/2$, i.e., half the mean distance between neighbouring impurities, we have:

$$\tan \frac{\theta_{min}}{2} = \frac{2Ze^2}{\varepsilon_o L} \Big/ \frac{m^* v^2}{2} \tag{3-31}$$

This gives the lower limit on the angular integration in (3-29). Here v is just the electron velocity because the electron mass, m^*, is much smaller than the impurity mass, M. From (3-30), we see that $\theta = 0$ corresponds to $b = \infty$, and which is not allowed when the impurity concentration is finite (Recall $L^{-3} \simeq n_D^{(+)}$), and that $\theta = \pi$ corresponds to $b = 0$(back scattering), we see the limitation on $\theta = \theta_{min} \neq 0$ necessarily. Letting $P_e = 2Ze^2/\varepsilon_o L$ for potential energy at the half spacing of impurities and $E_e = m^* v^2/2 = \hbar^2 k^2/2m^*$ for kinetic energy of an incident conduction electron, (3-31) gives:

$$\tan \frac{\theta_{min}}{2} = \frac{P_e}{E_e} \quad \text{or} \quad \frac{\sin^2 \frac{\theta_{min}}{2}}{1 - \sin^2 \frac{\theta_{min}}{2}} = \frac{P_e^2}{E_e^2}$$

Hence:

$$\sin^2 \frac{\theta_{min}}{2} = \left\{1 + \left(\frac{E_e}{P_e}\right)^2\right\}^{-1} = \tfrac{1}{2}\,(1 - \cos\theta_{min}) \qquad (3\text{-}32)$$

From (3-32), $\cos\theta_{min} \simeq 1$ for $E_e >> P_e$ gives $\theta_{min} \gtrsim 0$ (small angle scattering) but $\cos\theta_{min} \simeq -1$ for $E_e << P_e$ gives $\theta_{min} \simeq \pi$ (back scattering), so that small angle scattering will be predominant mainly at fairly high electron temperatures and low impurity concentrations.

3-4 General Form for Relaxation Time and Deduction of the Conwell-Weisskopf Result

From the small scattering angle, θ_{min}, we can calculate the reciprocal relaxation time, (3-29), due to the scattering from localized oscillating impurity atoms by use of (3-32). Before obtaining the general form we first obtain the Conwell-Weisskopf result by taking $\beta \to \infty$. Then (3-29) becomes:

$$\frac{1}{\tau_i^{c-w}} = \frac{2\pi Z^2 e^4 m^* n_D^{(+)}}{\varepsilon_o^2 \hbar^3 k^3} \int_{\theta=\theta_{min}}^{\pi} \frac{\sin\theta}{1 - \cos\theta}\, d\theta$$

$$= \frac{\pi Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2 (2m^*)^{\frac{1}{2}} E_e^{3/2}} \ln\left(1 + \frac{E_e^2}{P_e^2}\right) \qquad (3\text{-}33)$$

which is the exactly the result obtained by Conwell and Weisskopf assuming fixed scattering centres. To calculate (3-29), generally

we introduce a new variable, $X \equiv (1 - \cos\theta)k^2/\beta^2$. The upper and the lower limits of the integral in (3-29) are, respectively,

$$X_u = 2\frac{k^2}{\beta^2} \qquad (3\text{-}34\text{:a})$$

and

$$X_1 = (1 - \cos\theta_{min})\frac{k^2}{\beta^2} = \frac{2\frac{k^2}{\beta^2}}{1 + \frac{E_e^2}{P_e^2}} \qquad (3\text{-}34\text{:b})$$

so that the integral in (3-29) becomes:

$$\int_{\theta=\theta_{min}}^{\pi} \frac{\sin\theta}{1 - \cos\theta} e^{-(1-\cos\theta)\frac{k^2}{\beta^2}} d\theta \equiv \int_{X_1}^{X_u} \frac{e^{-X}}{X} dX \qquad (3\text{-}35)$$

We may evaluate (3-35) from tables of the exponential integral (see e.g., Arfken, (1970)); viz.,

$$E_i(x) = \int_x^{\infty} \frac{e^{-t}}{t} dt \qquad (3\text{-}36)$$

(3-35) may be given in terms of E_i; viz.,

$$\int_{X_1}^{X_u} \frac{e^{-X}}{X} dX = \int_{X_1}^{\infty} \frac{e^{-t}}{t} dt - \int_{X_u}^{\infty} \frac{e^{-t}}{t} dt = E_i(X_1) - E_i(X_u) \qquad (3\text{-}37)$$

but it is difficult to extract the functional dependence unless the

argument is very small or large.

Now consider the quantity, k^2/β^2; viz.,

$$\frac{k^2}{\beta^2} = \frac{\hbar k^2}{M\omega_o} = 2\,\frac{E_e}{\hbar\omega_o}\left(\frac{m^*}{M}\right) \tag{3-38}$$

where $E_e = \hbar^2 k^2/2m^*$ is the energy of an incident electron. From (3-38) we see that, unless ω_o is unusually small (assume $\omega_o \simeq 10^{13}\text{sec}^{-1}$) or E_e is particularly large (usually $E_e \simeq 10^{-14} \sim 10^{-13}$ erg), the quantity k^2/β^2, will be much less than unity since the ratio of an electron mass and an impurity mass is of the order of 10^{-5}. Hence in such a case we may expand the exponential term in the integral (3-35) to give:

$$\int_{X_l}^{X_u} \frac{e^{-X}}{X}\,dX = \ln\frac{X_u}{X_l} - (X_u - X_l) + \tfrac{1}{4}(X_u^2 - X_l^2) - \cdots\cdots\cdots$$

$$= \ln\left(1 + \frac{E_e^2}{P_e^2}\right) - \frac{2k^2}{\beta^2}\left(\frac{E_e^2/P_e^2}{1 + E_e^2/P_e^2}\right) + \cdots\cdots\cdots \tag{3-39}$$

where use has been made of (3-34:a,b), and $\beta^2 = M\omega_o/\hbar$.

From (3-29) and (3-39), the reciprocal of relaxation time for momentum transfer becomes:

$$\frac{1}{\tau_i} = \frac{\pi Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2 (2m^*)^{\frac{1}{2}} E_e^{3/2}} \left\{ \ln\left(1 + \frac{E_e^2}{P_e^2}\right) - \frac{2k^2}{\beta^2}\left(\frac{E_e^2/P_e^2}{1 + E_e^2/P_e^2}\right) + \cdots\cdots \right\} \tag{3-40}$$

where $E_e = \hbar^2 k^2/2m^*$ is the energy of the incident electron and $P_e = 2Ze^2/\varepsilon_o L = 2Ze^2 n_D^{(+)^{1/3}}/\varepsilon_o$ is the potential at half spacing of impurities. We see from (3-40) that if β goes to infinity, (3-40) leads to the Conwell-Weisskopf result.

(i) Fairly Low Temperatures and High Impurity Concentrations

In this case the condition, $E_e << P_e$, is satisfied, so that we can expand the logarithmic term in (3-40) to give:

$$\frac{1}{\tau_i} \simeq \frac{\pi Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2 (2m^*)^{1/2}} \cdot \frac{E_e^{1/2}}{P_e^2} \left\{ 1 - \frac{4E_e}{\frac{M}{m^*}\hbar\omega_o} + \cdots\cdots\cdots \right\}$$

We, therefore, have the relaxation time as:

$$\tau_i \simeq A E_e^{-1/2} (1 + B E_e + \cdots\cdots\cdots) \qquad (3\text{-}41\text{:a})$$

where:

$$\left[A = \frac{\varepsilon_o^2 (2m^*)^{1/2} P_e^2}{\pi Z^2 e^4 n_D^{(+)}} = \frac{4(2m^*)^{1/2}}{\pi\, n_D^{(+)1/3}} \right.$$

$$\left. B = \frac{4}{\frac{M}{m^*}\hbar\omega_o} \right.$$

If we assume the phonon temperature, $T_p \equiv \hbar\omega_o/k_B \simeq 200^{\circ}K$, electron temperature, T_e, of the order of 10^7, we have $BE_e \simeq 1$. Otherwise, BE_e is negligibly small.

(ii) Fairly High Temperatures and Low Impurity Concentration

In this case $E_e >> P_e$ holds and the reciprocal of the relaxation time, (3-40), is expressed by:

$$\frac{1}{\tau_i} \simeq \frac{2\pi Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2 (2m^*)^{1/2} E_e^{3/2}} \left\{ \ln\left(\frac{E_e}{P_e}\right) - \frac{2E_e}{\frac{M}{m^*}\hbar\omega_o} + \cdots\cdots \right\}$$

This leads to:

$$\tau_i \simeq C E_e^{3/2} (1 + D E_e + \cdots\cdots) \qquad (3\text{-}41\text{:}b)$$

where:

$$\left[C = \frac{\varepsilon_o^2 (2m^*)^{1/2}}{2\pi Z^2 e^4 n_D^{(+)} \ln(E_e/P_e)} \right.$$

$$\left. D = \frac{2}{\frac{M}{m^*}\hbar\omega_o \ln(E_e/P_e)} \right]$$

and the logarithmic term, $\ln(E_e/P_e)$, is slowly varying with $E_e \simeq KT_e$ (T_e: the electron temperature). Clearly DE_e must be comparable to unity if other than a $T^{3/2}$ dependence of mobility is to be observed, but this is unlikely since for all reasonable values of ω_o not in the spectrum of the lattice vibration it is clear that:

$$T_e << \tfrac{1}{2} \frac{M}{m^*} T_p \ln \frac{E_e}{P_e}$$

where $T_p \equiv \hbar\omega_o/k_B$ is the phonon temperature of the impurities. Assuming $T_p \simeq 200^{\circ}K$, as before, we find that for all temperatures $T_e << 10^8\ ^{\circ}K$, $DE_e << 1$.

We conclude from these results that an impurity with a localized mode widely separated from the normal lattice modes will not modify the Conwell-Weisskopf result appreciably.

PART II

Electron Scattering from Impurities Oscillating with Frequencies Common to Solvent Atoms

In semiconductors it is anticipated that most impurities will have masses and a force constant not widely different from those of the solvent atoms which make up the lattice, and consequently, in first approximation, they will oscillate with natural frequencies common to those of the solvent atoms. This means that we may not treat the impurity atoms as isolated harmonic oscillators as in Part I, but must include their dynamical properties with those of all the other crystal atoms.

To consider the scattering properties of such impurities, it is necessary, first, to establish the nature of the lattice vibration in the host crystal and in this section we therefore establish the form of the acoustic modes in a pure crystal and treat it as an isotropic, compressible medium. As is well known, such a formulation is valid at long wavelengths and should be adequate to give the order-of-magnitude of the effects we are considering.

4. The Lagrangian Formulation of a Lattice Field

In this chapter, we investigate the low frequency acoustical motion of the crystal and for this purpose we treat the lattice as a homogeneous, isotropic, elastic continuous medium characterized by a certain sound

velocity and macroscopic density. The procedure is to set up the classical field of an isotropic continuum. The equations of motion are then formed from the Lagrangian density and lead to the normal coordinates of the medium. These coordinates are collective in nature and in terms of them the total lattice Hamiltonian is a sum of squares; i.e., diagonal. Quantization is then straightforward and for this purpose we introduce field variables which are themselves creation and destruction operators for acoustic phonons.

To illustrate the Lagrangian procedure for handling the motion of continuous mechanical system, we shall seek the equations of motion for the longitudinal vibrations of a medium.

To this end, let $\underset{\sim}{\eta}(\underset{\sim}{R},t)$ be the small displacement of the medium at the point $\underset{\sim}{R} = (X,Y,Z)$ at a time t. If ρ_o is the undisturbed density of the medium, the kinetic energy density is:

$$T = \tfrac{1}{2} \rho_o \dot{\underset{\sim}{\eta}}^2 \qquad (4\text{-}1)$$

To obtain the potential energy density, let the mass of the medium be M, then the equilibrium volume is $V_o = M/\rho_o$ and if V is the potential energy density then VV_o represents the potential energy of the medium. As a result of a compressional disturbance, the volume changes from V_o to $V_o + \Delta V$. Now during a change in volume, dV, the work performed on the system, i.e., the increase in the potential energy is -PdV. Hence

the potential energy corresponding to a volume change from V_o to $V_o + \Delta V$ is:

$$V V_o = - \int_{V_o}^{V_o+\Delta V} P dV \qquad (4\text{-}2)$$

To evaluate (4-2), we expand the pressure, P, in a Taylor series about V_o and restrict ourselves to small changes in volume. Then we have:

$$P = P_o + \left(\frac{\partial P}{\partial V}\right)_{V=V_o} \Delta V + \cdots\cdots\cdots$$

so that (4-2) becomes:

$$V = - P_o \left(\frac{\Delta V}{V_o}\right) - \tfrac{1}{2} V_o \left(\frac{\partial P}{\partial V}\right)_{V=V_o} \left(\frac{\Delta V}{V_o}\right)^2 - \cdots\cdots\cdots \qquad (4\text{-}3)$$

Since the compressibility of a medium is defined by:

$$K_o \equiv - \frac{1}{V_o}\left(\frac{\partial V}{\partial P}\right)_o = - \frac{1}{\rho_o}\left(\frac{\partial \rho}{\partial P}\right)_{\rho_o} \qquad (4\text{-}4)$$

which is assumed known, (4-3) may be expressed in terms of the compressibility, (4-4):

$$V = - P_o \left(\frac{\Delta V}{V_o}\right) + \frac{1}{2K_o} \left(\frac{\Delta V}{V_o}\right)^2 - \cdots\cdots\cdots \qquad (4\text{-}5)$$

It is now convenient to eliminate ΔV in favour of the associated density change, $\Delta\rho$. Thus let:

$$\rho(\underset{\sim}{R},t) = \rho_o\{1 + \sigma(R,t)\}$$

where $\sigma(\underset{\sim}{R},t)$ is the fractional change in the density of the medium. Since $V = M/\rho$ the change in V is given by:

$$\Delta V = \Delta\left(\frac{M}{\rho}\right) = -\frac{M}{\rho_o^2}\Delta\rho = -V_o\,\sigma(\underset{\sim}{R},t)$$

so that (4-5) becomes:

$$V = P_o\sigma + \frac{1}{2K_o}\sigma^2 \qquad (4\text{-}6)$$

Finally we require to express σ in terms of the displacement, $\underset{\sim}{\eta}$. To do this, we employ the conservation of mass. Consider a closed surface, A, of any finite volume, V, in the medium. The mass flowing out of this volume due to a small disturbance from equilibrium is given by:

$$\delta M = \rho_o \int_A \underset{\sim}{\eta} \cdot d\underset{\sim}{A}$$

which is converted to the volume integral by use of Gauss' theorem:

$$\delta M = \rho_o \int_V \nabla \cdot \underset{\sim}{\eta} \, dV \tag{4-7}$$

δM is also given by:

$$\delta M = - \int_{V'} (\rho - \rho_o) \, dV = - \rho_o \int_{V'} \sigma \, dV \tag{4-8}$$

Since the equality holds for any arbitrary volume we must have from (4-7) and (4-8):

$$\sigma(\underset{\sim}{R},t) = - \nabla \cdot \underset{\sim}{\eta} \, (\underset{\sim}{R},t) \tag{4-9}$$

It is now seen that the term, $P_o \sigma = - P_o \nabla \cdot \underset{\sim}{\eta}$, can not contribute to the total potential energy of the medium since $\int_{V'} \nabla \cdot \underset{\sim}{\eta} \, dV = 0$ over a volume, V_o, being considered. Using this fact together with (4-9), the final form of the potential energy density, (4-6), for small disturbances is thus:

$$V = \frac{1}{2K_o} (\nabla \cdot \underset{\sim}{\eta})^2 \tag{4-10}$$

Using (4-1) and (4-10), the Lagrangian and the Hamiltonian densities are, respectively,

$$L = T - V = \tfrac{1}{2} \rho_o \{ \dot{\underset{\sim}{\eta}}^2 - S_o^2 (\nabla \cdot \underset{\sim}{\eta})^2 \} \tag{4-11:a}$$

$$H = T + V = \tfrac{1}{2} \rho_o \left\{ \dot{\underset{\sim}{\eta}}^2 + S_o^2 (\underset{\sim}{\nabla} \cdot \underset{\sim}{\eta})^2 \right\} \qquad (4\text{-}11\text{:}b)$$

where the sound speed in the medium is defined by:

$$S_o^2 \equiv \frac{1}{K_o \rho_o} \qquad (4\text{-}12)$$

The equations of motion follow from the Lagrangian density (Goldstein, (1950)):

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\eta}_i}\right) + \sum_{j=1}^{3} \frac{\partial}{\partial X_j} \left[\frac{\partial L}{\partial \left(\frac{\partial \eta_i}{\partial X_j}\right)} \right] - \frac{\partial L}{\partial \eta_i} = 0 \qquad (4\text{-}13)$$

From (4-11:a) and (4-13) we find:

$$\ddot{\underset{\sim}{\eta}}_i = S_o^2 \frac{\partial}{\partial X_i} (\underset{\sim}{\nabla} \cdot \underset{\sim}{\eta}) \qquad (4\text{-}14\text{:}a)$$

which may be combined into one vector equation as:

$$\ddot{\underset{\sim}{\eta}} = S_o^2 \underset{\sim}{\nabla} \cdot (\underset{\sim}{\nabla} \cdot \underset{\sim}{\eta}) \qquad (4\text{-}14\text{:}b)$$

Taking the divergence of both sides of (4-14:b) and using (4-9), we find:

$$\ddot{\sigma} = S_o^2 \nabla^2 \sigma \qquad (4\text{-}15)$$

where $\nabla^2 = \underset{\sim}{\nabla}\cdot\underset{\sim}{\nabla}$ is the Laplacian operator. (4-15) is the three dimensional acoustic wave equation with sound speed, S_o. We now note that a plane wave solution:

$$\underset{\sim}{\eta}(\underset{\sim}{R},t) \simeq \exp\{ i(\omega t + \underset{\sim}{q}\cdot\underset{\sim}{R})\}$$

leads to the well-known dispersion formula for the longitudinal acoustic waves; viz.,

$$\omega_q^2 = S_o^2 q^2 \qquad (4\text{-}16)$$

We note here that ω_q is a symmetric function of q and that, following Debye, $q \leq q_{max}$ is assumed to give the correct number of modes, q. Here q_{max} is the Debye cut-off wave number chosen so that the total number of acoustic modes equals three times the total number of particles in the crystal.

4-1 Normal Modes of Lattice

The Hamiltonian density and the total Hamiltonian of the system; viz.,

$$H = \tfrac{1}{2}\rho_o\{\dot{\underset{\sim}{\eta}}^2 + S_o^2(\underset{\sim}{\nabla}\cdot\underset{\sim}{\eta})^2\} \qquad (4\text{-}11\text{:b})$$

and

$$H_{lattice} = \int_{\underset{\sim}{R}} H \, d\underset{\sim}{R}^3 \tag{4-17}$$

are *not* a sum of squares of the generalized coordinates; $\dot{\underset{\sim}{\eta}}$ and $\underset{\sim}{\eta}$. To make the total energy diagonal we express them in terms of a new coordinates, i.e., the normal coordinates, which follow from the equations of motion; viz.,

$$\underset{\sim}{\eta}(\underset{\sim}{R},t) = \frac{1}{\sqrt{V_o}} \sum_{\underset{\sim}{q}} \underset{\sim}{\xi}_{\underset{\sim}{q}} Q_{\underset{\sim}{q}}(t) \, e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}} \tag{4-18}$$

where $\underset{\sim}{\xi}_{\underset{\sim}{q}}$ is the polalization vector parallel to $\underset{\sim}{\eta}$ for acoustic waves. The inverse of (4-18) is:

$$Q_{\underset{\sim}{q}}(t) = \frac{1}{\sqrt{V_o}} \int_{\underset{\sim}{R}} \underset{\sim}{\eta}(\underset{\sim}{R},t) \, e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}} \, d\underset{\sim}{R}^3 \tag{4-19}$$

where use has been made of the orthogonality result:

$$\int_{\underset{\sim}{R}} e^{i(\underset{\sim}{q}-\underset{\sim}{q}')\cdot\underset{\sim}{R}} \, d\underset{\sim}{R}^3 = V_o \, \delta_{\underset{\sim}{q},\underset{\sim}{q}'} \tag{4-20}$$

As defined by (4-18) the $Q_{\underset{\sim}{q}}$ are complex quantities and they have to satisfy the relations:

$$Q_{\underset{\sim}{q}}^{*} = Q_{-\underset{\sim}{q}} \tag{4-21}$$

in order that $\underset{\sim}{\eta}(\underset{\sim}{R},t)$ is real.

The $Q_{\underset{\sim}{q}}$ are the normal coordinates of the system and are essentially the Fourier amplitudes of the lattice displacement vector. From (4-19) they are seen to be collective in nature in that they depend on the sum of displacements at all points in the medium. We now see that the Hamiltonian is a sum of squares in terms of the $Q_{\underset{\sim}{q}}$: From (4-17), we find the total kinetic energy as:

$$T = \int_{\underset{\sim}{R}} T \, d\underset{\sim}{R}^3 = \tfrac{1}{2} \rho_o \int_{\underset{\sim}{R}} \dot{\underset{\sim}{\eta}}^2 d\underset{\sim}{R}^3 = \tfrac{1}{2} \rho_o \sum_{\underset{\sim}{q}} \dot{Q}_{\underset{\sim}{q}} \dot{Q}_{-\underset{\sim}{q}} \tag{4-22}$$

and the total potential energy as:

$$V = \int_{\underset{\sim}{R}} V d\underset{\sim}{R}^3 = \tfrac{1}{2} \rho_o S_o^2 \int_{\underset{\sim}{R}} (\nabla_{\underset{\sim}{\cdot}} \underset{\sim}{\eta})^2 \, d\underset{\sim}{R}^3 = \tfrac{1}{2} \rho_o S_o^2 \sum_{\underset{\sim}{q}} q^2 Q_{\underset{\sim}{q}} Q_{-\underset{\sim}{q}} \tag{4-23}$$

where use has been made of (4-18), (4-20) and (4-21). Hence from (4-22) and (4-23), we have the total Hamiltonian for lattice as:

$$H_{\text{lattice}} = T + V = \tfrac{1}{2} \rho_o \sum_{\underset{\sim}{q}} (\dot{Q}_{\underset{\sim}{q}} \dot{Q}_{-\underset{\sim}{q}} + \omega_q^2 Q_{\underset{\sim}{q}} Q_{-\underset{\sim}{q}}) \tag{4-24}$$

where use has been made of the dispersion relation (4-16).

Using (4-18) in (4-14:b), the equation of motion for the $Q_{\underset{\sim}{q}}$ are seen to be:

$$\underset{\sim}{\xi}_{\underset{\sim}{q}} \ddot{Q}_{\underset{\sim}{q}} + S_o^2 \underset{\sim}{q} (\underset{\sim}{\xi}_{\underset{\sim}{q}} \cdot \underset{\sim}{q}) Q_{\underset{\sim}{q}} = 0$$

or, scalar multiplying with $\underset{\sim}{q}$:

$$\ddot{Q}_{\underset{\sim}{q}}(t) + \omega_q^2 Q_{\underset{\sim}{q}}(t) = 0 \tag{4-25}$$

We see that the $Q_{\underset{\sim}{q}}(t)$ oscillate harmonically in time and that the crystal is thus equivalent to $3N_o$ independent harmonic oscillators.

4-2 Quantization of Lattice Field

Since the $Q_{\underset{\sim}{q}}$ are complex quantities it is necessary to define real amplitudes to quantize properly. Thus let

$$Q_{\underset{\sim}{q}} = \frac{1}{(2)^{\frac{1}{2}}} (u_{\underset{\sim}{q}} + i v_{\underset{\sim}{q}}) \tag{4-26}$$

so that we have:

$$Q_{-\underset{\sim}{q}} = \frac{1}{(2)^{\frac{1}{2}}} (u_{\underset{\sim}{q}} - i v_{\underset{\sim}{q}}) = Q_{\underset{\sim}{q}}^* \tag{4-27}$$

By use of (4-26) and (4-27), (4-24) becomes:

$$H_{\text{lattice}} = \tfrac{1}{2} \rho_o \sum_{\underset{\sim}{q}>0} \left\{ (\dot{u}_{\underset{\sim}{q}}^2 + \omega_q^2 u_{\underset{\sim}{q}}^2) + (\dot{v}_{\underset{\sim}{q}}^2 + \omega_q^2 v_{\underset{\sim}{q}}^2) \right\} \tag{4-28}$$

where the sum is taken over positive wave numbers, $\underset{\sim}{q}$.

We now define momenta canonically conjugate to $u_{\underset{\sim}{q}}$ and $v_{\underset{\sim}{q}}$ as:

$$\Pi_{\underset{\sim}{q}} \equiv \frac{\partial H_{lattice}}{\partial \dot{u}_{\underset{\sim}{q}}} = \rho_o \dot{u}_{\underset{\sim}{q}}; \qquad K_{\underset{\sim}{q}} \equiv \frac{\partial H_{lattice}}{\partial \dot{v}_{\underset{\sim}{q}}} = \rho_o \dot{v}_{\underset{\sim}{q}}$$

giving:

$$H_{lattice} = \sum_{\underset{\sim}{q}>0} \left\{ \frac{\Pi_{\underset{\sim}{q}}^2}{2\rho_o} + \tfrac{1}{2}\rho_o \omega_q^2 u_{\underset{\sim}{q}}^2 \right\} + \sum_{\underset{\sim}{q}>0} \left\{ \frac{K_{\underset{\sim}{q}}^2}{2\rho_o} + \tfrac{1}{2}\rho_o \omega_q^2 v_{\underset{\sim}{q}}^2 \right\} \qquad (4\text{-}29)$$

which corresponds *two* sets of oscillators since the $Q_{\underset{\sim}{q}}$ are complex.

Since $\Pi_{\underset{\sim}{q}}$ and $u_{\underset{\sim}{q}}$, and $K_{\underset{\sim}{q}}$ and $v_{\underset{\sim}{q}}$ are canonically conjugate variables, the system is quantized by requiring:

$$\begin{aligned} [u_{\underset{\sim}{q}}, \Pi_{\underset{\sim}{q}}] &\equiv u_{\underset{\sim}{q}}\Pi_{\underset{\sim}{q}} - \Pi_{\underset{\sim}{q}} u_{\underset{\sim}{q}} = i\hbar \\ [v_{\underset{\sim}{q}}, K_{\underset{\sim}{q}}] &\equiv v_{\underset{\sim}{q}} K_{\underset{\sim}{q}} - K_{\underset{\sim}{q}} v_{\underset{\sim}{q}} = i\hbar \end{aligned} \qquad (4\text{-}30)$$

In a Schördinger representation, (4-30) implies the momenta:

$$\Pi_{\underset{\sim}{q}} = -i\hbar \frac{\partial}{\partial u_{\underset{\sim}{q}}} \quad ; \qquad K_{\underset{\sim}{q}} = -i\hbar \frac{\partial}{\partial v_{\underset{\sim}{q}}} \qquad (4\text{-}31)$$

and substituting (4-31) into (4-29), the total lattice Hamiltonian becomes:

$$\begin{aligned} H_{lattice} &= \frac{\hbar^2}{2\rho_o} \sum_{\underset{\sim}{q}>0} \left(-\frac{\partial^2}{\partial u_{\underset{\sim}{q}}^2} + \alpha_{\omega_q}^2 u_{\underset{\sim}{q}}^2 \right) + \frac{\hbar^2}{2\rho_o} \sum_{\underset{\sim}{q}>0} \left(-\frac{\partial^2}{\partial v_{\underset{\sim}{q}}^2} + \alpha_{\omega_q}^2 v_{\underset{\sim}{q}}^2 \right) \\ &= \frac{\hbar^2}{2\rho_o} \sum_{\underset{\sim}{q}>0} \left\{ \left(-\frac{\partial}{\partial u_{\underset{\sim}{q}}} + \alpha_{\omega_q} u_{\underset{\sim}{q}} \right) \left(\frac{\partial}{\partial u_q} + \alpha_{\omega_q} u_{\underset{\sim}{q}} \right) + \alpha_{\omega_q} \right\} \\ &\quad + \frac{\hbar^2}{2\rho_o} \sum_{\underset{\sim}{q}>0} \left\{ \left(-\frac{\partial}{\partial v_{\underset{\sim}{q}}} + \alpha_{\omega_q} v_{\underset{\sim}{q}} \right) \left(\frac{\partial}{\partial v_{\underset{\sim}{q}}} + \alpha_{\omega_q} v_{\underset{\sim}{q}} \right) + \alpha_{\omega_q} \right\} \end{aligned} \qquad (4\text{-}32)$$

where $\alpha_{\omega_q} = \rho_o \omega_q / \hbar$

It is now desirable to make one final transformation from the real amplitudes, $u_{\underset{\sim}{q}}$ and $v_{\underset{\sim}{q}}$, of the normal coordinates to the field operators, $B_{\underset{\sim}{q}}$ and $B^{+}_{\underset{\sim}{q}}$, which act as destruction and creation operators for the field quanta (phonons). This transformation has been defined by Fröhlich, (1956) as:

$$B_{\underset{\sim}{q}} = \frac{1}{i(2)^{\frac{1}{2}}} \left(\sqrt{\alpha}_{\omega_q} Q_{\underset{\sim}{q}} + \frac{1}{\sqrt{\alpha}_{\omega_q}} \frac{\partial}{\partial Q_{-\underset{\sim}{q}}}\right)$$

$$B^{+}_{q} = \frac{1}{i(2)^{\frac{1}{2}}} \left(-\sqrt{\alpha}_{\omega_q} Q_{-\underset{\sim}{q}} + \frac{1}{\sqrt{\alpha}_{\omega_q}} \frac{\partial}{\partial Q_{\underset{\sim}{q}}}\right) \qquad (4\text{-}33)$$

and since $B^{+}_{\underset{\sim}{q}} \neq B_{-\underset{\sim}{q}}$ we have:

$$B_{-\underset{\sim}{q}} = \frac{1}{i(2)^{\frac{1}{2}}} \left(\sqrt{\alpha}_{\omega_q} Q_{-\underset{\sim}{q}} + \frac{1}{\sqrt{\alpha}_{\omega_q}} \frac{\partial}{\partial Q_{\underset{\sim}{q}}}\right)$$

$$B^{+}_{-\underset{\sim}{q}} = \frac{1}{i(2)^{\frac{1}{2}}} \left(-\sqrt{\alpha}_{\omega_q} Q_{\underset{\sim}{q}} + \frac{1}{\sqrt{\alpha}_{\omega_q}} \frac{\partial}{\partial Q_{-\underset{\sim}{q}}}\right) \qquad (4\text{-}34)$$

From these results the inverses are given by:

$$Q_{\underline{q}} = \frac{i}{\sqrt{2\alpha_{\omega_q}}} (B_{\underline{q}} - B^{+}_{-\underline{q}})$$
$$Q_{-\underline{q}} = \frac{i}{\sqrt{2\alpha_{\omega_q}}} (B_{-\underline{q}} - B^{+}_{\underline{q}}) \qquad (4\text{-}35)$$

and

$$\frac{\partial}{\partial Q_{\underline{q}}} = i\sqrt{\frac{\alpha_{\omega_q}}{2}}(B_{-\underline{q}} + B^{+}_{\underline{q}})$$
$$\frac{\partial}{\partial Q_{-\underline{q}}} = i\sqrt{\frac{\alpha_{\omega_q}}{2}}(B_{\underline{q}} + B^{+}_{-\underline{q}}) \qquad (4\text{-}36)$$

From (4-26) and (4-27) we find the inverses:

$$u_{\underline{q}} = \frac{1}{\sqrt{2}} (Q_{\underline{q}} + Q_{-\underline{q}})$$
$$v_{\underline{q}} = \frac{1}{i\sqrt{2}} (Q_{\underline{q}} - Q_{-\underline{q}}) \qquad (4\text{-}37)$$

so that from (4-35) we have (4-37) as:

$$u_{\underline{q}} = \frac{i}{2\sqrt{\alpha_{\omega_q}}} (B_{\underline{q}} + B_{-\underline{q}} - B^{+}_{\underline{q}} - B^{+}_{-\underline{q}})$$
$$v_{\underline{q}} = \frac{1}{2\sqrt{\alpha_{\omega_q}}} (B_{\underline{q}} - B_{-\underline{q}} + B^{+}_{\underline{q}} - B^{+}_{-\underline{q}}) \qquad (4\text{-}38)$$

Again, from (4-26) and (4-27) we find:

$$\frac{\partial}{\partial u_{\underset{\sim}{q}}} = \frac{\partial}{\partial Q_{\underset{\sim}{q}}} \cdot \frac{\partial Q_{\underset{\sim}{q}}}{\partial u_{\underset{\sim}{q}}} + \frac{\partial}{\partial Q_{-\underset{\sim}{q}}} \cdot \frac{\partial Q_{-\underset{\sim}{q}}}{\partial u_{\underset{\sim}{q}}} = \frac{1}{\sqrt{2}} \left(\frac{\partial}{\partial Q_{\underset{\sim}{q}}} + \frac{\partial}{\partial Q_{-\underset{\sim}{q}}}\right)$$

$$\frac{\partial}{\partial v_{\underset{\sim}{q}}} = \frac{\partial}{\partial Q_{\underset{\sim}{q}}} \cdot \frac{\partial Q_{\underset{\sim}{q}}}{\partial v_{\underset{\sim}{q}}} + \frac{\partial}{\partial Q_{-\underset{\sim}{q}}} \cdot \frac{\partial Q_{-\underset{\sim}{q}}}{\partial v_{\underset{\sim}{q}}} = \frac{i}{\sqrt{2}} \left(\frac{\partial}{\partial Q_{\underset{\sim}{q}}} - \frac{\partial}{\partial Q_{-\underset{\sim}{q}}}\right) \qquad (4\text{-}39)$$

so that from (4-36), we have (4-39) as:

$$\frac{\partial}{\partial u_{\underset{\sim}{q}}} = \frac{i}{2} \sqrt{\alpha_{\omega_q}} \left(B_{\underset{\sim}{q}} + B_{-\underset{\sim}{q}} + B^{+}_{\underset{\sim}{q}} + B^{+}_{-\underset{\sim}{q}}\right)$$

$$\frac{\partial}{\partial v_{\underset{\sim}{q}}} = \tfrac{1}{2} \sqrt{\alpha_{\omega_q}} \left(B_{\underset{\sim}{q}} - B_{-\underset{\sim}{q}} - B^{+}_{\underset{\sim}{q}} + B^{+}_{-\underset{\sim}{q}}\right) \qquad (4\text{-}40)$$

The results, (4-38) and (4-40), are now to be used in (4-32).

To express (4-32) in terms of the operators; $B_{\underset{\sim}{q}}$, $B_{-\underset{\sim}{q}}$, $B^{+}_{\underset{\sim}{q}}$ and $B^{+}_{-\underset{\sim}{q}}$, we first note that:

$$-\frac{\partial}{\partial u_{\underset{\sim}{q}}} + \alpha_{\omega_q} u_{\underset{\sim}{q}} = -i\sqrt{\alpha}_{\omega_q} \left(B^{+}_{\underset{\sim}{q}} + B^{+}_{-\underset{\sim}{q}}\right)$$

$$\frac{\partial}{\partial u_{\underset{\sim}{q}}} + \alpha_{\omega_q} u_{\underset{\sim}{q}} = i\sqrt{\alpha}_{\omega_q} \left(B_{\underset{\sim}{q}} + B^{+}_{-\underset{\sim}{q}}\right) \qquad (4\text{-}41)$$

$$-\frac{\partial}{\partial v_{\underset{\sim}{q}}} + \alpha_{\omega_q} v_{\underset{\sim}{q}} = \sqrt{\alpha}_{\omega_q} \left(B^{+}_{\underset{\sim}{q}} - B_{-\underset{\sim}{q}}\right)$$

$$\frac{\partial}{\partial v_{\underset{\sim}{q}}} + \alpha_{\omega_q} v_{\underset{\sim}{q}} = \sqrt{\alpha}_{\omega_q} \left(B_{\underset{\sim}{q}} - B_{-\underset{\sim}{q}}\right)$$

Hence by use of (4-41), (4-32) becomes :

$$H_{lattice} = \frac{\hbar^2}{2\rho_o} \sum_{\underset{\sim}{q}>0} \left\{ \alpha_{\omega_q} (B^+_{\underset{\sim}{q}} + B^+_{-\underset{\sim}{q}})(B_{\underset{\sim}{q}} + B_{-\underset{\sim}{q}}) + \alpha_{\omega_q} \right\}$$

$$+ \frac{\hbar^2}{2\rho_o} \sum_{\underset{\sim}{q}>0} \left\{ \alpha_{\omega_q} (B^+_{\underset{\sim}{q}} - B_{-\underset{\sim}{q}})(B_{\underset{\sim}{q}} - B_{-\underset{\sim}{q}}) + \alpha_{\omega_q} \right\}$$

$$= \tfrac{1}{2} \sum_{\underset{\sim}{q}>0} \hbar\omega_q \left\{ (B^+_{\underset{\sim}{q}} + B^+_{-\underset{\sim}{q}})(B_{\underset{\sim}{q}} + B_{-\underset{\sim}{q}}) + 1 \right\}$$

$$+ \tfrac{1}{2} \sum_{\underset{\sim}{q}>0} \hbar\omega_q \left\{ (B^+_{\underset{\sim}{q}} - B^+_{-\underset{\sim}{q}})(B_{\underset{\sim}{q}} - B_{-\underset{\sim}{q}}) + 1 \right\}$$

$$= \sum_{\underset{\sim}{q}>0} \hbar\omega_q \left\{ B^+_{\underset{\sim}{q}} B_{\underset{\sim}{q}} + \tfrac{1}{2} \right\} + \sum_{\underset{\sim}{q}>0} \hbar\omega_q \left\{ B^+_{-\underset{\sim}{q}} B_{-\underset{\sim}{q}} + \tfrac{1}{2} \right\}$$

$$= \sum_{\underset{\sim}{q}} \hbar\omega_{\underset{\sim}{q}} \left\{ B^+_{\underset{\sim}{q}} B_{\underset{\sim}{q}} + \tfrac{1}{2} \right\} \qquad (4\text{-}42)$$

This is the usual form for the energy arising from the field of $3N_o$ independent single harmonic oscillators.

4-3 Displacement Vector

We will express in this section a displacement vector of a lattice in terms of the operators; $B_{\underset{\sim}{q}}$ and $B^+_{\underset{\sim}{q}}$. For this purpose we shall use the results obtained in the previous sections. For each point in the medium we have introduced the displacement vector, $\underset{\sim}{\eta}(\underset{\sim}{R},t)$, that characterizes the displacement of the medium from its equilibrium position.

The displacement of the lattice at $\underset{\sim}{R}$ may be expressed by (4-18); viz.,

$$\underset{\sim}{\eta}(\underset{\sim}{R},t) = \frac{1}{(V_o)^{\frac{1}{2}}} \sum_{\underset{\sim}{q}} \underset{\sim}{\xi}_{\underset{\sim}{q}} Q_{\underset{\sim}{q}}(t)\, e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}}$$

but from (4-35), we have:

$$Q_{\underset{\sim}{q}} = \frac{i}{\sqrt{2\alpha}\,\omega_q}(B_{\underset{\sim}{q}} - B^{+}_{-\underset{\sim}{q}}) \; ; \qquad Q_{-\underset{\sim}{q}} = \frac{i}{\sqrt{2\alpha}\,\omega_q}(B_{-\underset{\sim}{q}} - B^{+}_{\underset{\sim}{q}})$$

Hence we can express $\underset{\sim}{\eta}(\underset{\sim}{R},t)$ in terms of the operators:

$$\begin{aligned}
\underset{\sim}{\eta}(\underset{\sim}{R},t) &= \frac{1}{(V_o)^{\frac{1}{2}}} \sum_{\underset{\sim}{q}>0} \underset{\sim}{\xi}_{\underset{\sim}{q}} \left\{ \frac{i}{\sqrt{2\alpha}\,\omega_q}(B_{\underset{\sim}{q}} - B^{+}_{-\underset{\sim}{q}}) e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}} \right\} \\
&\quad + \frac{1}{(V_o)^{\frac{1}{2}}} \sum_{\underset{\sim}{q}>0} \underset{\sim}{\xi}_{-\underset{\sim}{q}} \left\{ \frac{i}{\sqrt{2\alpha}\,\omega_q}(B_{-\underset{\sim}{q}} - B^{+}_{\underset{\sim}{q}}) e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}} \right\} \\
&= \frac{i}{\sqrt{2\alpha\,\omega_q\, V_o}} \sum_{\underset{\sim}{q}>0} \left[\underset{\sim}{\xi}_{\underset{\sim}{q}} (B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}}) - \underset{\sim}{\xi}_{\underset{\sim}{q}} (B_{-\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}} + B^{+}_{-\underset{\sim}{q}}\, e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}}) \right]
\end{aligned}$$

where use has been made of the property of the polarization vector,

$\underset{\sim}{\xi}_{-\underset{\sim}{q}} = -\,\underset{\sim}{\xi}_{\underset{\sim}{q}}$.

On reversing $\underset{\sim}{q}$ in the second term in the square bracket and noting $\underset{\sim}{\xi}_{-\underset{\sim}{q}} = -\,\underset{\sim}{\xi}_{\underset{\sim}{q}}$, we have:

$$\begin{aligned}
\underset{\sim}{\eta}(\underset{\sim}{R},t) &= \frac{i}{\sqrt{2\alpha\,\omega_q\, V_o}} \sum_{\underset{\sim}{q}>0} \underset{\sim}{\xi}_{\underset{\sim}{q}} (B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}}) \\
&\quad + \frac{i}{\sqrt{2\alpha\,\omega_q\, V_o}} \sum_{\underset{\sim}{q}<0} \underset{\sim}{\xi}_{\underset{\sim}{q}} (B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}})
\end{aligned}$$

Hence the displacement vector of the lattice at $\underset{\sim}{R}$ may be expressed by:

$$\underset{\sim}{\eta}(\underset{\sim}{R},t) = \frac{i}{\sqrt{2\alpha_{\omega_q} V_o}} \sum_{\underset{\sim}{q}} \underset{\sim}{\xi}_{\underset{\sim}{q}} \left(B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}}\right) \tag{4-43}$$

where $\alpha_{\omega_q} = \rho_o \omega_q/\hbar = \rho_o S_o q/\hbar$.

4-4 Commutation Rules for $B_{\underset{\sim}{q}}$ and $B^{+}_{\underset{\sim}{q}}$

It is important to obtain the main properties of the field operators; $B_{\underset{\sim}{q}}$ and $B^{+}_{\underset{\sim}{q}}$. The first of these follows from the basic commutation results, (4-30). Using (4-33), we find:

$$\left[B_{\underset{\sim}{q}},\ B^{+}_{\underset{\sim}{q}}\right] \equiv \left[\frac{1}{i\sqrt{2}}\left(\sqrt{\alpha_{\omega_q}}\, Q_{\underset{\sim}{q}} + \frac{1}{\sqrt{\alpha_{\omega_q}}}\cdot\frac{\partial}{\partial Q_{-\underset{\sim}{q}}}\right), \frac{1}{i\sqrt{2}}\left(\sqrt{\alpha_{\omega_q}}\, Q_{-\underset{\sim}{q}} + \frac{1}{\sqrt{\alpha_{\omega_q}}}\cdot\frac{\partial}{\partial Q_{\underset{\sim}{q}}}\right)\right]$$

$$= \frac{\alpha_{\omega_q}}{2}\left[Q_{\underset{\sim}{q}},\ Q_{-\underset{\sim}{q}}\right] + \frac{1}{2\alpha_{\omega_q}}\left[\frac{\partial}{\partial Q_{\underset{\sim}{q}}},\ \frac{\partial}{\partial Q_{-\underset{\sim}{q}}}\right] - \tfrac{1}{2}\left[Q_{\underset{\sim}{q}}, \frac{\partial}{\partial Q_{\underset{\sim}{q}}}\right] - \tfrac{1}{2}\left[Q_{-\underset{\sim}{q}}, \frac{\partial}{\partial Q_{-\underset{\sim}{q}}}\right]$$

but $\left[Q_{\underset{\sim}{q}},\ Q_{-\underset{\sim}{q}}\right] = 0$ since $Q_{\underset{\sim}{q}}^{*} = Q_{-\underset{\sim}{q}}$. Also we easily find, from (4-37), that:

$$\frac{\partial}{\partial Q_{\underset{\sim}{q}}} = \frac{\partial}{\partial u_{\underset{\sim}{q}}}\cdot\frac{\partial u_{\underset{\sim}{q}}}{\partial Q_{\underset{\sim}{q}}} + \frac{\partial}{\partial v_{\underset{\sim}{q}}}\cdot\frac{\partial v_{\underset{\sim}{q}}}{\partial Q_{\underset{\sim}{q}}} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial u_{\underset{\sim}{q}}} - i\,\frac{\partial}{\partial v_{\underset{\sim}{q}}}\right)$$

$$\frac{\partial}{\partial Q_{-\underset{\sim}{q}}} = \frac{\partial}{\partial u_{\underset{\sim}{q}}}\cdot\frac{\partial u_{\underset{\sim}{q}}}{\partial Q_{-\underset{\sim}{q}}} + \frac{\partial}{\partial v_{\underset{\sim}{q}}}\cdot\frac{\partial v_{\underset{\sim}{q}}}{\partial Q_{-\underset{\sim}{q}}} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial u_{\underset{\sim}{q}}} + i\,\frac{\partial}{\partial v_{\underset{\sim}{q}}}\right) \tag{4-44}$$

Hence we have:

$$\left[\frac{\partial}{\partial Q_{\underset{\sim}{q}}}, \frac{\partial}{\partial Q_{-\underset{\sim}{q}}}\right] = \left[\frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial u_{\underset{\sim}{q}}} - i\frac{\partial}{\partial v_{\underset{\sim}{q}}}\right), \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial u_{\underset{\sim}{q}}} + i\frac{\partial}{\partial v_{\underset{\sim}{q}}}\right)\right]$$

$$= \tfrac{1}{2}\left\{\left[\frac{\partial}{\partial u_{\underset{\sim}{q}}}, \frac{\partial}{\partial u_{\underset{\sim}{q}}}\right] + \left[\frac{\partial}{\partial v_{\underset{\sim}{q}}}, \frac{\partial}{\partial v_{\underset{\sim}{q}}}\right]\right.$$

$$\left. + i\left[\frac{\partial}{\partial u_{\underset{\sim}{q}}}, \frac{\partial}{\partial v_{\underset{\sim}{q}}}\right] - i\left[\frac{\partial}{\partial v_{\underset{\sim}{q}}}, \frac{\partial}{\partial u_{\underset{\sim}{q}}}\right]\right\} = 0$$

From (4-26) and (4-44) we find:

$$\left[Q_{\underset{\sim}{q}}, \frac{\partial}{\partial Q_{\underset{\sim}{q}}}\right] = \left[\frac{1}{\sqrt{2}}\left(u_{\underset{\sim}{q}} + iv_{\underset{\sim}{q}}\right), \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial u_{\underset{\sim}{q}}} - i\frac{\partial}{\partial v_{\underset{\sim}{q}}}\right)\right]$$

$$= \tfrac{1}{2}\left\{\left[u_{\underset{\sim}{q}}, \frac{\partial}{\partial u_{\underset{\sim}{q}}}\right] + \left[v_{\underset{\sim}{q}}, \frac{\partial}{\partial v_{\underset{\sim}{q}}}\right] - i\left[u_{\underset{\sim}{q}}, \frac{\partial}{\partial v_{\underset{\sim}{q}}}\right] + i\left[v_{\underset{\sim}{q}}, \frac{\partial}{\partial u_{\underset{\sim}{q}}}\right]\right\}$$

$$= -1$$

Similarly, from (4-27) and (4-44), we find:

$$\left[Q_{-\underset{\sim}{q}}, \frac{\partial}{\partial Q_{-\underset{\sim}{q}}}\right] = -1$$

Hence we find the commutation rule for $B_{\underset{\sim}{q}}$ and $B^{+}_{\underset{\sim}{q}}$ as:

$$\left[B_{\underset{\sim}{q}}, B^{+}_{\underset{\sim}{q}}\right] \equiv B_{\underset{\sim}{q}}B^{+}_{\underset{\sim}{q}} - B^{+}_{\underset{\sim}{q}}B_{\underset{\sim}{q}} = 1 \qquad (4\text{-}45)$$

Similarly, we may show that:

$$\left[B_{\underset{\sim}{q}} , B^{+}_{\underset{\sim}{q}'} \right] = 0 \qquad \text{for } \underset{\sim}{q}' \neq \underset{\sim}{q} \tag{4-46}$$

$$\left[B_{\underset{\sim}{q}} , B_{\underset{\sim}{q}'} \right] = \left[B^{+}_{\underset{\sim}{q}} , B^{+}_{\underset{\sim}{q}'} \right] = 0 \tag{4-47}$$

4-5 Property of $B_{\underset{\sim}{q}}$ and $B^{+}_{\underset{\sim}{q}}$

The property of the operators, $B_{\underset{\sim}{q}}$ and $B^{+}_{\underset{\sim}{q}}$, which make them particularly useful is that they are respectively destruction and creation operators. To see this, let us examine the eigenstates and the eigenvalues of the following engenvalue equation:

$$B^{+}_{\underset{\sim}{q}} B_{\underset{\sim}{q}} |\chi_{N_{\underset{\sim}{q}}}\rangle = \varepsilon_{N_{\underset{\sim}{q}}} |\chi_{N_{\underset{\sim}{q}}}\rangle$$

Using the commutation relation, (4-45), on

$$B_{\underset{\sim}{q}} \left(B^{+}_{\underset{\sim}{q}} B_{\underset{\sim}{q}}\right) |\chi_{N_{\underset{\sim}{q}}}\rangle = \varepsilon_{N_{\underset{\sim}{q}}} B_{\underset{\sim}{q}} |\chi_{N_{\underset{\sim}{q}}}\rangle$$

we get:

$$\left(B^{+}_{\underset{\sim}{q}} B_{\underset{\sim}{q}} + 1\right) B_{\underset{\sim}{q}} |\chi_{N_{\underset{\sim}{q}}}\rangle = \varepsilon_{N_{\underset{\sim}{q}}} B_{\underset{\sim}{q}} |\chi_{N_{\underset{\sim}{q}}}\rangle$$

or

$$B_{\underset{\sim}{q}}^{+} B_{\underset{\sim}{q}}(B_{\underset{\sim}{q}}|\chi_{N_{\underset{\sim}{q}}}\rangle) = (\varepsilon_{N_{\underset{\sim}{q}}} - 1) B_{\underset{\sim}{q}}|\chi_{N_{\underset{\sim}{q}}}\rangle$$

but:

$$B_{\underset{\sim}{q}}^{+} B_{\underset{\sim}{q}}|\chi_{N_{\underset{\sim}{q}}-1}\rangle = \varepsilon_{N_{\underset{\sim}{q}}-1}|\chi_{N_{\underset{\sim}{q}}}\rangle$$

so that we have:

$$\varepsilon_{N_{\underset{\sim}{q}}-1} = \varepsilon_{N_{\underset{\sim}{q}}} - 1 \; ; \quad B_{\underset{\sim}{q}}|\chi_{N_{\underset{\sim}{q}}}\rangle = \zeta|\chi_{N_{\underset{\sim}{q}}-1}\rangle$$

If $\varepsilon_{N_{\underset{\sim}{q}}} \equiv N_{\underset{\sim}{q}} = 0,1,2,\cdots\cdots$, we see that the eigenvalues are integers.

$$\langle\chi_{N_{\underset{\sim}{q}}}|B_{\underset{\sim}{q}}^{+} B_{\underset{\sim}{q}}|\chi_{N_{\underset{\sim}{q}}}\rangle = \zeta^{*}\zeta\langle\chi_{N_{\underset{\sim}{q}}-1}|\chi_{N_{\underset{\sim}{q}}-1}\rangle = |\zeta|^{2}\langle\chi_{N_{\underset{\sim}{q}}-1}|\chi_{N_{\underset{\sim}{q}}-1}\rangle$$

$$= N_{\underset{\sim}{q}}\langle\chi_{N_{\underset{\sim}{q}}}|\chi_{N_{\underset{\sim}{q}}}\rangle$$

but the states are orthonormalized so that we have

$$|\zeta|^{2} = N_{\underset{\sim}{q}}$$

Hence $\zeta = \sqrt{N_{\underset{\sim}{q}}} \times$ (Arbitrary phase factor). We, therefore, have the following equation:

$$B_{\underset{\sim}{q}}|\chi_{N_{\underset{\sim}{q}}}\rangle = \sqrt{N_{\underset{\sim}{q}}}\,|\chi_{N_{\underset{\sim}{q}}-1}\rangle \qquad (4\text{-}48)$$

It follows then that:

$$B_{\underset{\sim}{q}}^{+} B_{\underset{\sim}{q}} |\chi_{N_{\underset{\sim}{q}}}\rangle = N_{\underset{\sim}{q}} |\chi_{N_{\underset{\sim}{q}}}\rangle = \sqrt{N}_{\underset{\sim}{q}} B_{\underset{\sim}{q}}^{+} |\chi_{N_{\underset{\sim}{q}}-1}\rangle$$

and therefore:

$$B_{\underset{\sim}{q}}^{+} |\chi_{N_{\underset{\sim}{q}}}\rangle = \sqrt{N_{\underset{\sim}{q}} + 1}\, |\chi_{N_{\underset{\sim}{q}}+1}\rangle \tag{4-49}$$

We see from (4-48) and (4-49) that the $B_{\underset{\sim}{q}}$'s act to destroy a phonon with mode, $\underset{\sim}{q}$, and that the $B_{\underset{\sim}{q}}^{+}$'s act to create a phonon with mode, $\underset{\sim}{q}$. It follows that $B_{\underset{\sim}{q}}^{p}$ destroys p phonons and $B_{\underset{\sim}{q}}^{+p}$ creates p phonons:

$$\begin{aligned} B_{\underset{\sim}{q}}^{p} |\chi_p\rangle &= \sqrt{p!}\, |\chi_o\rangle \\ B_{\underset{\sim}{q}}^{+p} |\chi_o\rangle &= \sqrt{p!}\, |\chi_p\rangle \end{aligned} \tag{4-50}$$

Using these results, the energy and the state vector of the lattice Hamiltonian, (4-42), are:

$$E_{\underset{\sim}{n}} = \sum_{\underset{\sim}{q}} \hbar\omega_q \left(N_{\underset{\sim}{q}} + \tfrac{1}{2}\right) \tag{4-51}$$

$$|\chi_{\underset{\sim}{n}}\rangle = \prod_{\underset{\sim}{q}} |\chi_{N_{\underset{\sim}{q}}}\rangle \ , \tag{4-52}$$

respectively. Here $\omega_q = S_o q$, and $\underset{\sim}{n}$ with its components, $N_{\underset{\sim}{q}_j}$ ($j = 1,2,\cdots\cdots,3N_o$), represents the state of all $3N_o$ phonons comprising the medium.

5. The Model Hamiltonian of the System

In the light of the previous section, we now return to the problem of electron scattering from ionized impurities assuming these to oscillate at frequencies common with those of the pure, host crystal. Here we consider only acoustic modes.

If the equilibrium position of the ionized impurity centre is $\underset{\sim}{R}_i$ and its displacement at time t is $\underset{\sim}{\eta}_i(\underset{\sim}{R}_i,t)$, the Hamiltonian of the system (electron + ionized impurity + lattice) is:

$$H = H_{lattice} + H_{electron} + H_{int} \tag{5-1}$$

where:

$$H_{lattice} = \sum_{\underset{\sim}{q}} \hbar\omega_q \left(B^+_{\underset{\sim}{q}} B_{\underset{\sim}{q}} + \tfrac{1}{2}\right) \tag{5-2:a}$$

$$H_{electron} = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial \underset{\sim}{r}^2} \tag{5-2:b}$$

$$H_{int} = -\frac{Ze^2 e^{-k_D|\underset{\sim}{r}-\underset{\sim}{R}_i-\underset{\sim}{\eta}|}}{\varepsilon_o|\underset{\sim}{r}-\underset{\sim}{R}_i-\underset{\sim}{\eta}|} \tag{5-2:c}$$

where ε_o is the dielectric constant of the bulk material and $\underset{\sim}{r}$ and $\underset{\sim}{R}_i$ are the position vectors of a conduction electron and the ith ionized oscillating impurity atom, respectively. In (5-2:c) we have introduced the screened Coulomb potential where:

$$k_D^2 = \frac{4\pi n_o e^2}{\varepsilon_o k_B T_e} \tag{5-3}$$

is the Debye screening wave number, n_o being the average number density of conduction electrons. n_o is replaced by $Zn_D^{(+)}$ when all the impurities are ionized (in semiconductors at room temperature, this replacement is generally valid.).

As is well known, and as will be shown below, use of the screened potential (5-2:c) prevents the divergency in electron scattering at small angles discussed in Part I, 3. It is thus not necessary in this and subsequent sections to introduce any cut-off in the range of the interaction between the electron and ionized impurity.

6. Matrix Elements for Elastic Scattering

The matrix element for the scattering of a conduction electron from a state, $\underset{\sim}{k}$, to another, $\underset{\sim}{k}'$, due to the potential caused by the i^{th} ionized oscillating impurity whose vibrational state remains unchanged will be discussed by use of the Born approximation.

From (5-2:c), the matrix element for elastic scattering due to the potential caused by the i^{th} ionized oscillating impurity is:

$$\langle \underset{\sim}{nk}' | H_{int} | \underset{\sim}{nk} \rangle = \langle \chi_{\underset{\sim}{n}} | \int_{\underset{\sim}{r}} \frac{-Ze^2 e^{-k_D|\underset{\sim}{r}-\underset{\sim}{R}_i-\underset{\sim}{n}|}}{\varepsilon_o V_o |\underset{\sim}{r}-\underset{\sim}{R}_i-\underset{\sim}{n}|} e^{i(\underset{\sim}{k}-\underset{\sim}{k}')\cdot\underset{\sim}{r}} d\underset{\sim}{r}^3 | \chi_{\underset{\sim}{n}} \rangle \tag{6-1}$$

where $|\underset{\sim}{n}\ \underset{\sim}{k}\rangle$ is the state vector of the unperturbed Hamiltonian; $H_{lattice} + H_{electron}$, and is given by:

$$|\underset{\sim}{n}\ \underset{\sim}{k}\rangle = |\underset{\sim}{n}\rangle|\underset{\sim}{k}\rangle \tag{6-2}$$

where:

$$|\underset{\sim}{n}\rangle \equiv |\chi_{\underset{\sim}{n}}\rangle = \prod_{\underset{\sim}{q}} |\chi_{N_{\underset{\sim}{q}}}\rangle \tag{6-2:a}$$

for the lattice and

$$|\underset{\sim}{k}\rangle = \frac{1}{\sqrt{V_o}} \exp\ (i\underset{\sim}{k}\cdot\underset{\sim}{r}) \tag{6-2:b}$$

for the conduction electron.

Letting $\underset{\sim}{K} = \underset{\sim}{k} - \underset{\sim}{k}'$ be the change in the wave number of the conduction electron on scattering, and $\underset{\sim}{\rho}_i = \underset{\sim}{r} - \underset{\sim}{R}_i - \underset{\sim}{n}$ its relative coordinate with respect to the i^{th} impurity centre, the matrix element, (6-1), is re-written as:

$$\langle \underset{\sim}{n}\underset{\sim}{k}'|H_{int}|\underset{\sim}{n}\underset{\sim}{k}\rangle = -\frac{Ze^2}{\varepsilon_o V_o}\int_{\mathcal{L}_i} \frac{e^{-k_D\rho_i}\, e^{i\underset{\sim}{K}\cdot\underset{\sim}{\rho}_i}}{\rho_i}\, d\underset{\sim}{\rho}_i^{\,3} \langle \chi_{\underset{\sim}{n}}| e^{i\underset{\sim}{K}\cdot(\underset{\sim}{R}_i+\underset{\sim}{n})} |\chi_{\underset{\sim}{n}}\rangle$$

$$= -\frac{4\pi Ze^2}{\varepsilon_o V_o(K^2+k_D^{\,2})} \left\{ e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}_i} \langle \chi_{\underset{\sim}{n}}| e^{i\underset{\sim}{K}\cdot\underset{\sim}{n}} |\chi_{\underset{\sim}{n}}\rangle \right\} \tag{6-3}$$

where, from (4-43), the displacement of the i^{th} impurity centre may be expressed by:

$$\underset{\sim}{\eta}(\underset{\sim}{R}_i) = \frac{i}{\sqrt{2\alpha_{\omega_q} V_o}} \sum_{\underset{\sim}{q}} \underset{\sim}{\xi}_{\underset{\sim}{q}} \left\{ B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} \right\} \tag{6-4}$$

with $\alpha_{\omega_q} = \rho_o \omega_q/\hbar = \rho_o S_o q/\hbar$.

By use of (6-4), we obtain:

$$i\underset{\sim}{K}\cdot\underset{\sim}{\eta} = \frac{i}{\sqrt{2\alpha_{\omega_q} V_o}} \sum_{\underset{\sim}{q}} i\underset{\sim}{K}\cdot\underset{\sim}{\xi}_{\underset{\sim}{q}} \left\{ B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} \right\} \tag{6-5}$$

In the above expression $i\underset{\sim}{K}\cdot\underset{\sim}{\eta}$ must be pure imaginary. It is, thus, convenient to include the factor $i = \sqrt{-1}$ with the phase factor; $i = e^{i\pi/2}$. Introducing $\overline{\underset{\sim}{q}\cdot\underset{\sim}{R}_i} = \underset{\sim}{q}\cdot\underset{\sim}{R}_i + \pi/2$, we obtain (6-5) as:

$$i\underset{\sim}{K}\cdot\underset{\sim}{\eta} = i \sum_{\underset{\sim}{q}} \frac{\underset{\sim}{K}\cdot\underset{\sim}{\xi}_{\underset{\sim}{q}}}{\sqrt{2\alpha_{\omega_q} V_o}} \left\{ B_{\underset{\sim}{q}} e^{i\overline{\underset{\sim}{q}\cdot\underset{\sim}{R}_i}} + B^{+}_{\underset{\sim}{q}} e^{-i\overline{\underset{\sim}{q}\cdot\underset{\sim}{R}_i}} \right\} \tag{6-6}$$

Since $B_{\underset{\sim}{q}}$ and $B^{+}_{\underset{\sim}{q}}$ operate only the lattice state, $|\chi_{N_{\underset{\sim}{q}}}\rangle$, we find, using (6-6), that the lattice part of the matrix element, (6-3), becomes:

$$\langle \chi_{\underset{\sim}{\eta}} | e^{i\underset{\sim}{K}\cdot\underset{\sim}{\eta}} | \chi_{\underset{\sim}{\eta}} \rangle = \prod_{\underset{\sim}{q}} \left\{ \langle \chi_{N_{\underset{\sim}{q}}} | \exp \left[iW_{\underset{\sim}{q}} \left(B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} \right) \right] | \chi_{N_{\underset{\sim}{q}}} \rangle \right\} \tag{6-7}$$

where we have dropped the "bar" notation and

$$W_{\underset{\sim}{q}} \equiv \frac{\underset{\sim}{K}\cdot\underset{\sim}{\xi}_{\underset{\sim}{q}}}{\sqrt{2\alpha_{\omega_q} V_o}} = \sqrt{\frac{\hbar K^2}{2\rho_o V_o S_o q}}\,(\underset{\sim}{\xi}_{\underset{\sim}{K}} \cdot \underset{\sim}{\xi}_{\underset{\sim}{q}}) \qquad (6\text{-}8)$$

with $\underset{\sim}{\xi}_{\underset{\sim}{K}}$ being the unit vector in the recoil direction $\underset{\sim}{K} = \underset{\sim}{k} - \underset{\sim}{k}'$.

The quantity, $W_{\underset{\sim}{q}}$, is a measure of the "recoilessness" of the scattering. When $W_{\underset{\sim}{q}}$ goes to zero as when $M = \rho_o V_o$ (total mass of the bulk material) is large, the scattering is purelly coulombic as from a stationary impurity. Since $W_{\underset{\sim}{q}}$ can be made arbitrarily small, we may expand the exponential in (6-7), as:

$$\exp\left\{ iW_{\underset{\sim}{q}} \left(B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i}\right) \right\} = \sum_{n=0}^{\infty} \frac{(-1)^n W_{\underset{\sim}{q}}^{2n}}{(2n)!}\, A^{2n}_{\text{elastic}} \qquad (6\text{-}9)$$

where:

$$A^{2n}_{\text{elastic}} = \left(B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i}\right)^{2n} \qquad (6\text{-}10)$$

We have restricted the sum in (6-9) to be taken over only even powers since odd powers lead to a net creation or destruction of acoustic phonons and hence to inelastic scattering which is of no interest here.

We now have to find the general form for the expectation values of the transition matrix of A^{2n}_{elastic} : i.e.,

$$A^{2n}_{\text{elastic}} = \left(B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i}\right)^{2n} \equiv \left(B_{\underset{\sim}{q}} + B^{+}_{\underset{\sim}{q}}\right)^{2n}$$

This final expression is valid for elastic cases because of the even

power of the bracket, but only terms that have equal numbers of operators of the $B_{\underset{\sim}{q}}$'s and the $B^{+}_{\underset{\sim}{q}}$'s need be taken into account for elastic scattering. The general form for the expectation value of $A^{2n}_{elastic}$ (see Appendix A) is:

$$\langle \chi_{N_{\underset{\sim}{q}}} | A^{2n}_{elastic} | \chi_{N_{\underset{\sim}{q}}} \rangle = \sum_{r=0}^{n} \frac{(2n)!\,2^r}{2^n (r!)^2 (n-r)!} \cdot \frac{N_{\underset{\sim}{q}}!}{(N_{\underset{\sim}{q}}-r)!} \qquad (6\text{-}11)$$

where n = 0,1,2·····. It is significant to note that the coefficient of the highest power of $N_{\underset{\sim}{q}}$ is given by:

$$\frac{(2n)!}{(n!)^2} \qquad (6\text{-}11\text{:a})$$

while the constant term is given by:

$$\frac{(2n)!}{2^n\, n!} \qquad (6\text{-}11\text{:b})$$

If we appeal to the assumption that $W_{\underset{\sim}{q}}$ is small (recall that the crystal mass is essentially infinite), we may restrict our interest to small values of n in (6-9). From (6-11), we have:

(i) for n = 0

$$\langle \chi_{N_{\underset{\sim}{q}}} | A^{0}_{elastic} | \chi_{N_{\underset{\sim}{q}}} \rangle = 1$$

(ii) For n = 1

$$\langle \chi_{N_{\underset{\sim}{q}}} | A^2_{\text{elastic}} | \chi_{N_{\underset{\sim}{q}}} \rangle = 2N_{\underset{\sim}{q}} + 1$$

(iii) For n = 2

$$\langle \chi_{N_{\underset{\sim}{q}}} | A^4_{\text{elastic}} | \chi_{N_{\underset{\sim}{q}}} \rangle = 6N_{\underset{\sim}{q}}^2 + 6N_{\underset{\sim}{q}} + 3$$

(iv) For n = 3

$$\langle \chi_{N_{\underset{\sim}{q}}} | A^6_{\text{elastic}} | \chi_{N_{\underset{\sim}{q}}} \rangle = 20N_{\underset{\sim}{q}}^3 + 30N_{\underset{\sim}{q}}^2 + 40N_{\underset{\sim}{q}} + 15$$

etc., so that from (6-9) we may have the following form for the full elastic scattering processes; viz.,

$$\begin{aligned}
&\langle \chi_{N_{\underset{\sim}{q}}} | \exp\left\{ iW_{\underset{\sim}{q}} \left(B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^+_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} \right) \right\} | \chi_{N_{\underset{\sim}{q}}} \rangle \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n W_{\underset{\sim}{q}}^{2n}}{(2n)!} \langle \chi_{N_{\underset{\sim}{q}}} | A^{2n}_{\text{elastic}} | \chi_{N_{\underset{\sim}{q}}} \rangle \\
&\simeq 1 - \frac{W_{\underset{\sim}{q}}^2}{2!}(2N_{\underset{\sim}{q}} + 1) + \frac{W_{\underset{\sim}{q}}^4}{4!}(6N_{\underset{\sim}{q}}^2 + 6N_{\underset{\sim}{q}} + 3) - \frac{W_{\underset{\sim}{q}}^6}{6!}(20N_{\underset{\sim}{q}}^3 + 30N_{\underset{\sim}{q}}^2 + 40N_{\underset{\sim}{q}} + 15) + \cdots\cdots
\end{aligned} \tag{6-12}$$

Reordering the powers of $N_{\underset{\sim}{q}}$, (6-12) may be written as:

$$\langle \chi_{N_q} | \exp\{ iW_q \cdot (B_q e^{iq\cdot R_i} + B_q^+ e^{-iq\cdot R_i}) \} | \chi_{N_q} \rangle$$

$$= \left[1 - \left(\frac{W_q^2}{2}\right) + \frac{1}{2}\left(\frac{W_q^2}{2}\right)^2 - \frac{1}{3}\left(\frac{W_q^2}{2}\right)^3 + \cdots\cdots\cdots \right]$$

$$- W_q^2 N_q \left[1 - \frac{W_q^2}{4} + \frac{W_q^4}{18} - \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \right]$$

$$+ \tfrac{1}{4} W_q^4 N_q^2 \left[1 - \frac{W_q^2}{6} + \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \right]$$

$$- \frac{3}{100} W_q^6 N_q^3 \left[1 - \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \right]$$

$$+ \cdots\cdots\cdots \qquad (6\text{-}13)$$

where:

$$W_q = \sqrt{\frac{\hbar K^2}{2\rho_o V_o S_o q}}\,(\xi_K \cdot \xi_q) \text{ with } K = k - k'$$

6-1 Absolute Zero Temperature

At the absolutely zero of temperature, $T = o^{\circ}K$, N_q is zero. Hence (6-13) reduces to the first set of square brackets and may be expressed by:

$$\langle \chi_o | \exp\{ iW_q \cdot (B_q e^{iq\cdot R_i} + B_q^+ e^{-iq\cdot R_i}) \} | \chi_o \rangle$$

$$= 1 - \frac{W_q^2}{2} + \frac{1}{2!}\left(\frac{W_q^2}{2}\right)^2 - \frac{1}{3!}\left(\frac{W_q^2}{2}\right)^3 + \cdots\cdots \simeq \exp(-W_q^2/2) \qquad (6\text{-}14)$$

6-2 Low Temperatures

At very low temperatures, $N_{\underset{\sim}{q}} \ll 1$. Hence the matrix, (6-13), reduces approximately to the first two terms of (6-12) and may be written as:

$$\langle \chi_{N_q} | \exp \{ i W_{\underset{\sim}{q}} \cdot (B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i}) \} | \chi_{N_{\underset{\sim}{q}}} \rangle \simeq \exp \left\{ -W_{\underset{\sim}{q}}^{2} (1+2N_{\underset{\sim}{q}})/2 \right\} \tag{6-15}$$

which leads to (6-14) when $T = 0^{\circ}K$ (i.e., $N_{\underset{\sim}{q}} = 0$).

We note here that the Gaussian expressions, (6-14) and (6-15), represent the well-known Debye-Waller factor for the reduction in the cross section for the scattering of a plane wave from a crystal - the excess momentum being taken up by the whole lattice. For γ-ray emission from a radioactive impurity in a crystal, (6-14) and (6-15) lead to the Mössbaur effect. It represents the fraction of events which occur without recoil (if $W_{\underset{\sim}{q}} = 0$ there is no recoil), and hence leads to extremely narrow line widths when $W_{\underset{\sim}{q}}$ is small. In X-ray diffraction, (6-14) and (6-15) lead to the fraction of such recoilless scatterings, and in neutron diffraction to the fraction of recoilless scatterings or capture possible for a given neutron energy.

In our problem the Debye-Waller factor will lead to the fraction of conduction electrons which scatter from ionized oscillating impurity

centres without recoil; the recoil being taken up by the acoustic phonons. The Conwell-Weisskopf (1950) and the Brooks-Herring formulae (unpublished) are based on a model in which this factor is assumed to be unity (i.e., infinitely massive scattering centres lead to fully recoilless scattering). What we do here is to estimate what reduction from unity is to be expected in the practical case.

6-3 High Temperatures

At high temperatures, $N_{\underset{\sim}{q}} >> 1$ holds. Hence each of the matrix elements will be characterized essentially by the terms with the highest power of $N_{\underset{\sim}{q}}$; viz.,

$$\langle \chi_{N_{\underset{\sim}{q}}} | A^{2n}_{\text{elastic}} | \chi_{N_{\underset{\sim}{q}}} \rangle = \langle \chi_{N_{\underset{\sim}{q}}} | (B_{\underset{\sim}{q}} + B^{+}_{\underset{\sim}{q}})^{2n} | \chi_{N_{\underset{\sim}{q}}} \rangle \simeq \frac{(2n)!}{(n!)^2} N_{\underset{\sim}{q}}{}^{n} \qquad (6\text{-}16)$$

Hence the matrix, (6-12), may be expressed by:

$$\langle \chi_{N_{\underset{\sim}{q}}} | \exp \{ i W_{\underset{\sim}{q}} \cdot (B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i}) \} | \chi_{N_{\underset{\sim}{q}}} \rangle \simeq \sum_{n=0}^{\infty} \frac{(-1)^n W_{\underset{\sim}{q}}{}^{2n}}{(n!)^2} N_{\underset{\sim}{q}}{}^{n} \qquad (6\text{-}17)$$

We note here that the series expansion for the zero-order Bessel function is:

$$J_o(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\frac{x}{2}\right)^{2n} \qquad (6\text{-}18)$$

Hence (6-17) may be written:

$$\langle \chi_{N_{\underset{\sim}{q}}} | \exp\{ i W_{\underset{\sim}{q}} \cdot (B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i}) \} | \chi_{N_{\underset{\sim}{q}}} \rangle \simeq J_o(2W_{\underset{\sim}{q}} N_{\underset{\sim}{q}}^{\frac{1}{2}}) \qquad (6\text{-}19)$$

From the results, (6-14), (6-15), (6-19) and (6-7), the scattering matrix, (6-3), may be expressed in the following form ; viz.,

$$\langle \underset{\sim}{n}\underset{\sim}{k}' | H_{int} | \underset{\sim}{n}\underset{\sim}{k} \rangle = - \frac{4\pi Ze^2}{\varepsilon_o V_o (K^2 + k_D^2)} e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}_i} \prod_{\underset{\sim}{q}} D_{\underset{\sim}{q}} \qquad (6\text{-}20)$$

where the Debye-Waller factor, $D_{\underset{\sim}{q}}$, is defined by:

$$D_{\underset{\sim}{q}} = \begin{cases} \exp\left\{-W_{\underset{\sim}{q}}^2 (1 + 2N_{\underset{\sim}{q}})/2\right\} & \text{for very low temperatures} \quad (N_{\underset{\sim}{q}} << 1) \qquad (6\text{-}21\text{:a}) \\ J_o(2W_{\underset{\sim}{q}} N_{\underset{\sim}{q}}^{\frac{1}{2}}) & \text{for high temperatures} \quad (N_{\underset{\sim}{q}} >> 1) \qquad (6\text{-}21\text{:b}) \end{cases}$$

and $W_{\underset{\sim}{q}}$ is given by (6-8) and J_o is the zero-order Bessel function given by (6-18)

7. Relaxation Time for Momentum Transfer (Elastic Case)

We have obtained the scattering matrix in the previous chapter. The probability of a transition per unit time can be obtained by use of it. Since the perturbation theory gives for the transition rate from i to f:

$$P_{i\to f} = \frac{2\pi}{\hbar}|\langle f|H_{int}|i\rangle|^2\,\delta(E_f - E_i) \tag{7-1}$$

the transition probability rate that a conduction electron will be scattered from a state, k, to another, k', due to the potential caused by the i^{th} ionized impurity, but the lattice state remains unchanged is given from (6-20) and (7-1):

$$P_{\underset{\sim}{nk}\to\underset{\sim}{nk}'} = \frac{2\pi}{\hbar}\,K_{\underset{\sim}{nk}'}|H_{int}|_{\underset{\sim}{nk}}\rangle|^2\,\delta(E_{\underset{\sim}{nk}'} - E_{\underset{\sim}{nk}})$$

$$= \frac{32\pi^3 Z^2 e^4}{\varepsilon_o^{\,2} V_o^{\,2}(K^2+k_D^{\,2})^2}\,(\prod_{\underset{\sim}{q}} D_{\underset{\sim}{q}})^2\,\delta(E_{\underset{\sim}{nk}'} - E_{\underset{\sim}{nk}}) \tag{7-2}$$

Assuming that the all scattering events by oscillating ionized impurities are independent we then find the total transition probability rate by summing (7-2) over all impurities, viz.,

$$P^{T}_{\underset{\sim}{nk}\to\underset{\sim}{nk}'} = \sum_{i=1}^{N_D^{(+)}} P_{\underset{\sim}{nk}\to\underset{\sim}{nk}'} = \frac{32\pi^3 Z^2 e^4 n_D^{(+)}}{\hbar\varepsilon_o^{\,2} V_o (K^2+k_D^{\,2})^2}\,(\prod_{\underset{\sim}{q}} D_{\underset{\sim}{q}})^2\,\delta(E_{\underset{\sim}{nk}'} - E_{\underset{\sim}{nk}}) \tag{7-3}$$

where $\underset{\sim}{K} = \underset{\sim}{k} - \underset{\sim}{k}'$ is the momentum change that the conduction electron suffers on scattering and $n_D^{(+)} = N_D^{(+)}/\,V_o$ is the ionized impurity density. The initial and the final energy of the system are, respectively:

$$E_{\underset{\sim}{nk}} = \frac{\hbar^2 k^2}{2m^*} + \sum_{\underset{\sim}{q}} \hbar\omega_q\,(N_{\underset{\sim}{q}} + \tfrac{1}{2}) \tag{7-4:a}$$

$$E_{\underset{\sim}{nk}'} = \frac{\hbar^2 k'^2}{2m^*} + \sum_{\underset{\sim}{q}} \hbar\omega_q\,(N_{\underset{\sim}{q}} + \tfrac{1}{2}) \tag{7-4:b}$$

We see that the δ-function ensures the energy conservation of the system,and thus from (7-4:a,b), it follows that:

$$k = k' \tag{7-5}$$

We must now sum (7-3) over all final electronic states to find the relaxation time, keeping in mind the distribution function of the conduction electrons for semiconductors follows the Boltzmann statistics.

We take the electronic distribution function, $f(\underset{\sim}{k})$, to be a pure number such that:

$$\frac{V_o}{8\pi^3} f(\underset{\sim}{k})\, d\underset{\sim}{k}^3 \tag{7-6}$$

is the number of electrons having wave numbers between $\underset{\sim}{k}$ and $\underset{\sim}{k}+d\underset{\sim}{k}$. Now the linear momentum of the conduction electron in this range is:

$$\underset{\sim}{M}(\underset{\sim}{k}) = \hbar \underset{\sim}{k}\, f(\underset{\sim}{k}) \tag{7-7}$$

Since in a simple scattering event, an electron in a state, $\underset{\sim}{k}$, initially will change its momentum by an amount, $\Delta\underset{\sim}{p}(\underset{\sim}{k}) = \hbar(\underset{\sim}{k}-\underset{\sim}{k}')$, the total rate of loss of momentum by the electrons in the state, $\underset{\sim}{k}$, through interaction with one or another of the ionized oscillating impurities is given by:

$$\left.\frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t}\right]_{loss} = -\sum_{\underset{\sim}{k}'} \hbar(\underset{\sim}{k}-\underset{\sim}{k}')\, f(\underset{\sim}{k}) \left\{1 - f(\underset{\sim}{k}')\right\} P^{T}_{n\underset{\sim}{k}\rightarrow n\underset{\sim}{k}'} \qquad (7\text{-}8)$$

where $1 - f(\underset{\sim}{k}')$ is the probability that the final state, $\underset{\sim}{k}'$, is unoccupied. In a similar way we may find the total rate of gain of momentum by electrons in the state, $\underset{\sim}{k}$, through scattering from all possible states, $\underset{\sim}{k}'$, by the processes in question to be:

$$\left.\frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t}\right]_{gain} = \sum_{\underset{\sim}{k}'} \hbar(\underset{\sim}{k}-\underset{\sim}{k}')\, f(\underset{\sim}{k}') \left\{1 - f(\underset{\sim}{k})\right\} P^{T}_{n\underset{\sim}{k}'\rightarrow n\underset{\sim}{k}} \qquad (7\text{-}9)$$

From (7-8) and (7-9) the net rate of gain of momentum by electrons between $\underset{\sim}{k}$ and $\underset{\sim}{k}+d\underset{\sim}{k}$ may be given by:

$$\left.\frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t}\right]_{net} = \left.\frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t}\right]_{gain} + \left.\frac{\partial \underset{\sim}{M}(\underset{\sim}{k})}{\partial t}\right]_{loss}$$

$$= \sum_{\underset{\sim}{k}'} \hbar(\underset{\sim}{k}-\underset{\sim}{k}') \left\{ f(\underset{\sim}{k}') - f(\underset{\sim}{k})\right\} P^{T}_{n\underset{\sim}{k}\rightarrow n\underset{\sim}{k}'} \qquad (7\text{-}10)$$

where we have used the principle of microscopic reversibility; viz., $P_{i\rightarrow f} = P_{f\rightarrow i}$ (P is a transition probability rate).

From (7-7) and (7-10) the rate of change of the distribution for the conduction electrons relevant to momentum transfer by the elastic scattering processes is, thus:

$$\frac{\partial f(\underset{\sim}{k})}{\partial t} = A(\underset{\sim}{k}) - B(\underset{\sim}{k}) \cdot f(\underset{\sim}{k}) \qquad (7\text{-}11)$$

where:

$$A(\underset{\sim}{k}) = \sum_{\underset{\sim}{k}'} (1 - \underset{\sim}{k}'\cdot\underset{\sim}{k}/k^2)\ P^{T}_{\underset{\sim}{nk}\rightarrow\underset{\sim}{nk}'}\ f(\underset{\sim}{k}') \tag{7-12:a}$$

$$B(\underset{\sim}{k}) = \sum_{\underset{\sim}{k}'} (1 - \underset{\sim}{k}'\cdot\underset{\sim}{k}/k^2)\ P^{T}_{\underset{\sim}{nk}\rightarrow\underset{\sim}{nk}'} \tag{7-12:b}$$

As in chapter 3, the standard technique for formulating the concept of the relaxation time is to treat $A(\underset{\sim}{k})$ as a slowly varying function of time since $B(\underset{\sim}{k})$ is time-independent. Then (7-10) may be integrated to give:

$$f(\underset{\sim}{k}) = f^{o}(\underset{\sim}{k}) + \zeta\, e^{-B(\underset{\sim}{k})t} \tag{7-13}$$

where $f^{o}(\underset{\sim}{k})$ is the equilibrium distribution function, and $B(\underset{\sim}{k})$ is the reciprocal of the relaxation time; viz.,

$$\frac{1}{\tau_i} = \sum_{\underset{\sim}{k}'} (1 - \underset{\sim}{k}'\cdot\underset{\sim}{k}/k^2)\ P^{T}_{\underset{\sim}{nk}\rightarrow\underset{\sim}{nk}'} \tag{7-14}$$

where we may replace the sum over all the final states, k', by an integral using the density of states function, viz.,

$$\sum_{\underset{\sim}{k}'} (\cdots\cdots) = \frac{V_o}{8\pi^3}\int_{\underset{\sim}{k}'} (\cdots\cdots)\, d\underset{\sim}{k}'^{3} \tag{7-15}$$

We, therefore, have (7-14) as:

$$\frac{1}{\tau_i} = \frac{V_o}{8\pi^3}\int_{\underset{\sim}{k}'} (1 - \underset{\sim}{k}'\cdot\underset{\sim}{k}/k^2)\ P^{T}_{\underset{\sim}{nk}\rightarrow\underset{\sim}{nk}'}\, d\underset{\sim}{k}'^{3}$$

or employing (7-3), the reciprocal of the relaxation time is given by:

$$\frac{1}{\tau_i} = \frac{4Z^2e^4n_D^{(+)}}{\hbar\varepsilon_o^2}\int_{\underset{\sim}{k}'} \frac{1-\underset{\sim}{k}'\cdot\underset{\sim}{k}/k^2}{|(\underset{\sim}{k}-\underset{\sim}{k}')^2+k_D^2|^2}\,(\pi D_{\underset{\sim}{q}})^2\,\delta(E_{n\underset{\sim}{k}'}-E_{n\underset{\sim}{k}})\,d\underset{\sim}{k}'^3 \qquad (7\text{-}16)$$

where the Debye-Waller factor, $D_{\underset{\sim}{q}}$, is given by (6-21:a,b).

We first evaluate (7-16) by integrating over the magnitude of $\underset{\sim}{k}'$ to get rid of the δ-function. Since from (7-4:a,b)

$$d(E_{n\underset{\sim}{k}'}-E_{n\underset{\sim}{k}}) = d\left(\frac{\hbar^2k'^2}{2m^*}-\frac{\hbar^2k^2}{2m^*}\right) = \frac{\hbar^2}{m^*}\,\underset{\sim}{k}'\cdot d\underset{\sim}{k}'$$

we have:

$$k'^2dk' = \frac{m^*}{\hbar^2}\,k'd(E_{n\underset{\sim}{k}'}-E_{n\underset{\sim}{k}})\,. \qquad (7\text{-}17)$$

Without loss of generality we can let $\underset{\sim}{k}$ lie along the Z-axis so that $\underset{\sim}{k}'$ makes an angle, $\theta_{\underset{\sim}{k}'}$, with $\underset{\sim}{k}$. Since $d\underset{\sim}{k}'^3 = k'^2dk'd\Omega_{\underset{\sim}{k}'}$, using (7-17), (7-16) becomes:

$$\frac{1}{\tau_i} = \frac{4Z^2e^4m^*n_D^{(+)}}{\hbar^3\varepsilon_o^2}\int_{\Omega_{\underset{\sim}{k}'}} \frac{1-\underset{\sim}{k}'\cdot\underset{\sim}{k}/k^2}{|(\underset{\sim}{k}-\underset{\sim}{k}')^2+k_D^2|^2}\,(\pi D_{\underset{\sim}{q}})^2\,k'\,\delta(E_{n\underset{\sim}{k}'}-E_{n\underset{\sim}{k}})$$
$$\times d(E_{n\underset{\sim}{k}'}-E_{n\underset{\sim}{k}})\quad d\Omega_{\underset{\sim}{k}'} \qquad (7\text{-}18)$$

where $d\Omega_{\underset{\sim}{k}'} = \sin\theta_{\underset{\sim}{k}'}\,d\theta_{\underset{\sim}{k}'}d\phi_{\underset{\sim}{k}'}$ is the differential solid angle and here

$(\theta_{\underset{\sim}{k}'}, \phi_{\underset{\sim}{k}'})$ are the polar and the azimuthal angle of $\underset{\sim}{k}'$. We first integrate (7-18) about the energy part. Keeping in mind that, due to the δ-function, only $k' = k$ contributes to the integral, the general form for the reciprocal of relaxation time, (7-18), is given by:

$$\frac{1}{\tau_i} = \frac{Z^2 e^4 m^* n_D^{(+)}}{\varepsilon_o^2 \hbar^3 k^3} \int_{\Omega_{\underset{\sim}{k}}} \frac{1 - \cos\theta_{\underset{\sim}{k}}}{\left\{1-\cos\theta_{\underset{\sim}{k}}+k_D^2/2k^2\right\}^2} (\Pi D_{\underset{\sim}{q}})^2_{k'=k} \, d\Omega_{\underset{\sim}{k}} \qquad (7\text{-}19)$$

where the Debye-Waller factor, $D_{\underset{\sim}{q}}$, must be evaluated for $k' = k$ at which $W_{\underset{\sim}{q}}$ is given by:

$$W_{\underset{\sim}{q}} = \sqrt{\frac{\hbar k^2}{2\rho_o V_o S_o q}} (\cos\theta_{\underset{\sim}{q}} - \cos\theta_{\underset{\sim}{k},\underset{\sim}{q}}) \qquad (7\text{-}20\text{:a})$$

with $\cos\theta_{\underset{\sim}{k},\underset{\sim}{q}} = \cos\theta_{\underset{\sim}{k}}\cos\theta_{\underset{\sim}{q}} + \sin\theta_{\underset{\sim}{k}}\sin\theta_{\underset{\sim}{q}}\cos(\phi_{\underset{\sim}{q}} - \phi_{\underset{\sim}{q}})$ (7-20:b)

7-1 The Conwell-Weisskopf Formula

From the general form for the reciprocal relaxation time due to the Mössbauer type scattering, we can deduce the Conwell-Weisskopf (1950) formula. To show this, we assume that $D_{\underset{\sim}{q}} = 1$ for all $\underset{\sim}{q}$, i.e., we assume that all scattering events take place without recoil or - what amounts to the same thing - that the phonons remove the excess momentum completely and distribute it over the whole lattice so that the solvent atoms and the impurity atoms remain fixed. Taking $k_D = 0$, which corresponds to no screening by conduction electrons, (7-19), after integrating over $\phi_{\underset{\sim}{k}}$, becomes:

$$\frac{1}{\tau_i^{C-W}} = \frac{2\pi Z^2 e^4 m^* n_D^{(+)}}{\varepsilon_o^2 \hbar^3 k^3} \int \frac{\sin\theta_{\underset{\sim}{k}}}{1 - \cos\theta_{\underset{\sim}{k}}} \, d\theta_{\underset{\sim}{k}} \qquad (7\text{-}21)$$

which exhibits the divergency at a lower limit, $\theta_{\underset{\sim}{k}} = 0$; the well-known "Coulomb divergency". In a plasma of ionized impurity atoms and conduction electrons at finite concentration, it is clear that scattering angle, $\theta_{\underset{\sim}{k}} = 0$, can not exist since it corresponds to scattering events which take place at infinite distances from the impurity centre and such can not occur at finite concentrations because of interference from the next-nearest neighbour impurity. Hence in practice $\theta_{\underset{\sim}{k}}$ has a lower limit, θ_{min}, determined by the impact parameter, b, which is of the order of half the average distance between scattering centres; $2b = L \simeq (n_D^{(+)})^{-\frac{1}{3}}$. Determination of the lower limit of the integral was given in chapter 3. Letting $\theta_{\underset{\sim}{k}} = \theta_{min}$ for the lower limit of the integral in (7-21), and using

the result of (3-32), we have the Conwell-Weisskopf formula:

$$\frac{1}{\tau_i^{C-W}} = \frac{\pi Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2 (2m^*)^{\frac{1}{2}} E_e^{3/2}} \ln\left(1 + \frac{E_e^2}{P_e^2}\right) \tag{7-22}$$

where $E_e = \hbar^2 k^2/2m^*$ and $P_e = 2Ze^2/\varepsilon_o L$ are the kinetic energy of an incident electron and the potential energy at a half distance of impurity spacing, L/2, respectively.

7-2 The Brooks-Herring Formula

The Brooks-Herring formula is essentially the same as the Conwell-Weisskopf formula. Here one takes account of the screening effect of electrons: The result follows from (7-19) assuming that $D_{\underset{\sim}{q}} = 1$ for all $\underset{\sim}{q}$. For this case we can readily integrate (7-19) over the solid angle $\Omega_{\underset{\sim}{k}}$ to give the Brooks-Herring result:

$$\frac{1}{\tau_i^{B-H}} = \frac{2\pi Z^2 e^4 m^* n_D^{(+)}}{\varepsilon_0^2 \hbar^3 k^3} \int_{\theta_{\underset{\sim}{k}}=0}^{\pi} \frac{1 - \cos\theta_{\underset{\sim}{k}}}{\left\{1 - \cos\theta_{\underset{\sim}{k}} + k_D^2/2k^2\right\}^2} \sin\theta_{\underset{\sim}{k}} d\theta_{\underset{\sim}{k}}$$

$$= \frac{\pi Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2 (2m^*)^{\frac{1}{2}} E_{\underset{\sim}{k}}^{3/2}} \left[\ln(1 + b) - \frac{b}{1 + b}\right] \tag{7-23}$$

where $b \equiv \frac{4k^2}{k_D^2} = 4\frac{E_{\underset{\sim}{k}}}{E_D}$ (7-24)

and $E_{\underset{\sim}{k}} = \hbar^2 k^2/2m^*$ is the energy of an incident electron and $E_D = \hbar^2 k_D^2/2m^*$ is the Debye energy of an incident electron with wavenumber equal to the Debye wave number. The Debye wave number, k_D, is given by (5-3).

7-3 Relaxation Time for Mössbaur Type Scattering

To evaluate relaxation time due to the Mössbaur type impurity scattering, (7-19), we have to calculate the Debye-Waller factor at $k' = k$.

(i) Low Temperatures ($N_{\underset{\sim}{q}} \ll 1$)

For very low temperatures, the Debye-Waller factor is given by (6-21:a), from which we have:

$$(\Pi D_{\underset{\sim}{q}\,\underset{\sim}{q}})^2 = \exp\left\{-\sum_{\underset{\sim}{q}} W_{\underset{\sim}{q}}^{\,2}\,(1 + 2N_{\underset{\sim}{q}})\right\} \tag{7-25}$$

We may replace the summation over all phonon modes, $\underset{\sim}{q}$, by an integral introducing the density of lattice states, $\rho(\underset{\sim}{q})$, via.,

$$\sum_{\underset{\sim}{q}} (\cdots\cdots\cdots) = \int_{\underset{\sim}{q}} (\cdots\cdots\cdots)\rho(\underset{\sim}{q})\, d\underset{\sim}{q}^3 \tag{7-26}$$

where in the Debye theory $\rho(\underset{\sim}{q})$ is given by:

$$\rho(\underset{\sim}{q})\, d\underset{\sim}{q}^3 = \frac{3V_o}{8\pi^3}\, d\underset{\sim}{q}^3 \tag{7-27}$$

which implies that the medium is isotropic so that one longitudinal mode and two transverse acoustic modes are taken into account. According

to the Debye theory, the maximum wave number that the medium can propagate is found by the condition that the total number of modes equals three times the number of lattice atoms, N_o, in the medium; viz.,

$$3No = \int_0^{q_{max}} \rho(\underset{\sim}{q})\, d\underset{\sim}{q}^3 = \frac{3V_o}{8\pi^3} \int_0^{q_{max}} d\underset{\sim}{q}^3 = \frac{V_o}{2\pi^2}\, q_{max}^3$$

Hence:

$$q_{max} = \left(\frac{6\pi^2 N_o}{V_o}\right)^{1/3} = (6\pi^2 n_o)^{1/3} \tag{7-28}$$

Employing (7-26) and (7-27) to calculate the power of the exponential in (7-25) and from (7-20:a), we have:

$$\sum_{\underset{\sim}{q}} W_{\underset{\sim}{q}}^2 (1+2N_{\underset{\sim}{q}}) = \frac{3V_o}{8\pi^3} \int_{\underset{\sim}{q}} W_{\underset{\sim}{q}}^2 (1+2N_{\underset{\sim}{q}})\, d\underset{\sim}{q}^3$$

$$= \frac{3\hbar k^2}{16\pi^3 \rho_o S_o} \int_{\Omega_{\underset{\sim}{q}}} (\cos\theta_{\underset{\sim}{q}} - \cos\theta_{\underset{\sim}{k},\underset{\sim}{q}})^2\, d\Omega_{\underset{\sim}{q}} \int_q (1+2N_{\underset{\sim}{q}}) q\, dq \tag{7-29}$$

where $d\Omega_{\underset{\sim}{q}} = \sin\theta_{\underset{\sim}{q}}\, d\theta_{\underset{\sim}{q}}\, d\phi_{\underset{\sim}{q}}$.

Since the average number of acoustic phonons, $N_{\underset{\sim}{q}}$, is independent of angles, $\theta_{\underset{\sim}{q}}$ and $\phi_{\underset{\sim}{q}}$, we can integrate (7-29) over the angular part by use of (7-20 :b)

$$\int_{\Omega_{\underset{\sim}{q}}} (\cos\theta_{\underset{\sim}{q}} - \cos\theta_{\underset{\sim}{k},\underset{\sim}{q}})^2 \, d\Omega_{\underset{\sim}{q}} = \frac{8\pi}{3} (1 - \cos\theta_{\underset{\sim}{k}}) \tag{7-30}$$

Hence, from (7-30), (7-29) becomes:

$$\sum_{\underset{\sim}{q}} W_{\underset{\sim}{q}}^2 (1 + 2N_{\underset{\sim}{q}}) = \frac{\hbar k^2 (1-\cos\theta_{\underset{\sim}{k}})}{2\pi^2 \rho_o S_o} \int_0^{q_{max}} (1 + \frac{2}{e^{\hbar S_o q/k_B T} - 1}) \, q \, dq$$

where use has been made of the Planck distribution function for phonon number; viz.,

$$N_{\underset{\sim}{q}} = \left[\exp(\hbar S_o q/k_B T) - 1 \right]^{-1} \tag{7-31}$$

Letting $u \equiv \hbar S_o q/k_B T$ and introducing the Debye temperature, Θ, of the bulk material by the relation, $\hbar S_o q_{max} = k_B \Theta$, we have:

$$\sum_{\underset{\sim}{q}} W_{\underset{\sim}{q}}^2 (1+2N_{\underset{\sim}{q}}) = \frac{\hbar k^2}{2\pi^2 \rho_o S_o} (1-\cos\theta_{\underset{\sim}{k}}) (\frac{k_B T}{\hbar S_o})^2 \int_0^{\Theta/T} (1 + \frac{2}{e^u - 1}) u \, du$$

$$= \frac{3\hbar^2 k^2 N_o}{2k_B \Theta} \left\{ 1 + \frac{2}{3} \pi^2 (\frac{T}{\Theta})^2 \right\} (1 - \cos\theta_{\underset{\sim}{k}}) \tag{7-32}$$

where use has been made of $q_{max}^3 = 6\pi^2 N_o / V_o$ and

$$\int_0^{\infty} \frac{u}{e^u - 1} \, du = \frac{\pi^2}{6} .$$

The approximation to the upper limit is valid since for very low temperatures $T << \Theta$. Defining:

$$\beta_{\underset{\sim}{k}} \equiv \frac{3E_{\underset{\sim}{k}}}{k_B\Theta} \frac{m^*}{(M/N_o)} \left\{ 1 + \frac{2}{3}\pi^2\left(\frac{T}{\Theta}\right)^2 \right\} \tag{7-33}$$

(7-32) can be written in terms of $\beta_{\underset{\sim}{k}}$ and then (7-25) can be written as:

$$(\pi D_{\underset{\sim}{q}})^2_{k'=k} = \exp\left\{-\beta_{\underset{\sim}{k}}(1 - \cos\theta_{\underset{\sim}{k}})\right\} \tag{7-34}$$

Substitution of (7-34) into (7-19) gives the reciprocal of relaxation time for the Mössbauer type ionized impurity scattering at very low temperatures:

$$\frac{1}{\tau_i} = \frac{2\pi Z^2 e^4 m^* n_D^{(+)}}{\varepsilon_o^2 \hbar^3 k^3} \int_{\theta_{\underset{\sim}{k}}} \frac{1 - \cos\theta_{\underset{\sim}{k}}}{\left\{1-\cos\theta_{\underset{\sim}{k}}+k_D^2/2k^2\right\}^2} e^{-\beta_{\underset{\sim}{k}}(1-\cos\theta_{\underset{\sim}{k}})} \sin\theta_{\underset{\sim}{k}}\, d\theta_{\underset{\sim}{k}} \tag{7-35}$$

It is important to note that (7-35) differs from the Brooks-Herring result (see(7-23)) only through the exponential factor $\exp\left\{-\beta(1-\cos\theta_{\underset{\sim}{k}})\right\}$ in the integral.

(ii) <u>High Temperatures</u> ($N_{\underset{\sim}{q}} >> 1$)

For high temperatures, the Debye-Waller factor is given by (6-21:b) and for phonon number, $N_{\underset{\sim}{q}}$, we can use the high temperature approximation; viz.,

$$N_{\underset{\sim}{q}} = \left[\exp(\hbar S_o q/k_B T) - 1\right]^{-1} \simeq \frac{k_B T}{\hbar S_o q} \tag{7-36}$$

Since series expansion of the zero-order Bessel function is:

$$J_o(x) = 1 - (\frac{x}{2})^2 + \frac{1}{2^2}(\frac{x}{2})^4 - \frac{1}{6^2}(\frac{x}{2})^6 + \cdots\cdots\cdots$$

we have:

$$J_o^2(x) = 1 - \frac{1}{2}x^2 + \frac{3}{32}x^4 - \frac{5}{576}x^6 + \cdots\cdots\cdots$$

On the other hand;

$$e^{-x^2/2} = 1 - \frac{1}{2}x^2 + \frac{1}{8}x^4 - \frac{1}{48}x^6 + \cdots\cdots\cdots$$

Hence for small value of the argument of J_o we may approximate $J_o^2(x)$ as:

$$J_o^2(x) \leq e^{-x^2/2}$$

and there results:

$$(\Pi D_{\underset{\sim}{q}})^2 \leq \exp\left\{-2 \sum_{\underset{\sim}{q}} W_{\underset{\sim}{q}}^2 N_{\underset{\sim}{q}}\right\}. \qquad (7\text{-}37)$$

We note here that this approximation can be made as precise as desired by choosing the volume V_o sufficiently large. Comparing (7-37) with (7-25) we see that at very low temperatures ($T \leq 1^oK$) one phonon process is very signigicant. For semiconductors, except for very low temperatures, we can use (7-36) as the phonon distribution and we may, therefore,

neglect unity compared with $2N_{\underset{\sim}{q}}$ in the round bracket in (7-25). This leads to the expression, (7-37). To calculate (7-37) we introduce the density of lattice states and employ the phonon distribution, (7-36). We then have the power of the exponential in (7-37) as:

$$\sum_{\underset{\sim}{q}} W_{\underset{\sim}{q}}^2 N_{\underset{\sim}{q}} = \frac{3V_o}{8\pi^3}\int_{\underset{\sim}{q}} W_{\underset{\sim}{q}}^2 N_{\underset{\sim}{q}}\, d\underset{\sim}{q}^3$$

$$= \frac{3k^2 k_B T}{16\pi^3 \rho_o S_o^2}\iint_{q\,\Omega_{\underset{\sim}{q}}} (\cos\theta_{\underset{\sim}{q}} - \cos\theta_{\underset{\sim}{k},\underset{\sim}{q}})^2\, dq\, d\Omega_{\underset{\sim}{q}} \qquad (7\text{-}38)$$

where use has been made of (7-20:a). The angular part of the integral in (7-38) is exactly the same as (7-30). Hence (7-38) can be written as:

$$\sum_{\underset{\sim}{q}} W_{\underset{\sim}{q}}^2 N_{\underset{\sim}{q}} = \frac{k^2 k_B T}{2\pi^2 \rho_o S_o^2}(1 - \cos\theta_{\underset{\sim}{k}}) \int_0^{q_{max}} dq$$

$$= \frac{3\hbar^2 k^2 N_o}{M k_B \Theta}\left(\frac{T}{\Theta}\right)(1 - \cos\theta_{\underset{\sim}{k}}) \qquad (7\text{-}39)$$

where we have used the relation, $\hbar S_o q_{max} = k_B\Theta$ and $q_{max}^3 = 6\pi^2 N_o/V_o$

Defining:

$$\beta'_{\underset{\sim}{k}} \equiv 12\,\frac{E_{\underset{\sim}{k}}}{k_B\Theta}\,\frac{m^*}{(M/N_o)}\,\frac{T}{\Theta} \qquad (7\text{-}40)$$

(7-38) can be written in terms of $\beta'_{\underset{\sim}{k}}$ and then (7-37) can be written as:

$$(\pi D_{\underset{\sim}{q}})^2_{k'=k} = \exp\left\{-\beta'_{\underset{\sim}{k}}\,(1 - \cos\theta_{\underset{\sim}{k}})\right\} \qquad (7\text{-}41)$$

Substituting (7-41) into (7-19), we have the reciprocal of relaxation time for the Mössbauer type ionized impurity scattering at high temperatures:

$$\frac{1}{\tau_i} = \frac{2\pi Z^2 e^4 m^* n_D^{(+)}}{\varepsilon_o^2 \hbar^3 k^3} \int_{\theta_{\underset{\sim}{k}}} \frac{1 - \cos\theta_{\underset{\sim}{k}}}{\left\{1 - \cos\theta_{\underset{\sim}{k}} + k_D^2/2k^2\right\}^2} e^{-\beta'_{\underset{\sim}{k}}(1-\cos\theta_{\underset{\sim}{k}})} \sin\theta_{\underset{\sim}{k}} \, d\theta_{\underset{\sim}{k}} \tag{7-42}$$

where now $\beta'_{\underset{\sim}{k}}$ is given by (7-40).

7-4 Change in Relaxation Time for Elastic Recoilless Scattering

To obtain the explicit forms of (7-35) and (7-42), we have to calculate the following integral:

$$\int_0^2 \frac{X \, e^{-cX}}{(X + a)^2} \, dX \tag{7-43}$$

where $X = 1 - \cos\theta_{\underset{\sim}{k}}$, $a = k_D^2/2k^2$ and $c = \beta_{\underset{\sim}{k}}$ for low temperatures and $\beta'_{\underset{\sim}{k}}$ for high temperatures are given by (7-33) and (7-40), respectively. The lower and the upper limits of the integral, (7-43), take 0 and 2, corresponding to $\theta_{\underset{\sim}{k}} = 0$ and π, respectively.

This integral, (7-43), may be evaluated exactly from tables of the exponential integral for any given c. However, for our purposes c is, practically, bound to be small for both $\beta_{\underset{\sim}{k}}$ and $\beta'_{\underset{\sim}{k}}$. Since $T < \Theta$, it is clear, because of the small ratio, $m^*/(M/N_o) \simeq 10^{-5}$, that $E_{\underset{\sim}{k}} >> k_B\Theta$ for both $\beta_{\underset{\sim}{k}}$ and $\beta'_{\underset{\sim}{k}}$ to be comparable to unity. This indicates a need for hot electrons in media of low Debye temperature for significant recoil scattering to occur. Setting $E_{\underset{\sim}{k}} = 3k_BT_e/2$ and $T_e/\Theta \simeq 10^1 \sim 10^2$, we see both $\beta_{\underset{\sim}{k}}$ $\beta'_{\underset{\sim}{k}} \simeq 10^{-4} \sim 10^{-3}$ and, accordingly, we may expand the exponential in (7-43) to give:

$$\int_0^2 \frac{X\, e^{-cx}}{(X+a)^2}\, dX = \int_0^2 \frac{X}{(X+a)^2}\,(1 - cX + \cdots\cdot)dX$$

$$= \{\ln(1+\frac{2}{a}) - \frac{2/a}{1+2/a}\} + 2ac\{\ln(1+\frac{2}{a}) - \frac{2+2/a}{2+a}\} + \cdots$$

(7-44)

where $c = \beta_{\underset{\sim}{k}}$ for low temperatures and $\beta'_{\underset{\sim}{k}}$ for high temperatures are given by (7-33) and (7-40), respectively and $a = k_D^2/2k^2$.

(i) Low Temperatures ($N_{\underset{\sim}{q}} << 1$)

For very low temperatures, from (7-35) and (7-44) we have the reciprocal of relaxation time for the Mössbauer type ionized impurity scattering as:

$$\frac{1}{\tau_i} = \frac{\pi Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2 (2m^*)^{\frac{1}{2}} E_{\underset{\sim}{k}}^{3/2}} \left[\{ \ln(1+b) - \frac{b}{1+b} \} + 4 \frac{c}{b} \{ \ln(1+b) - \frac{1 + b/2}{1 + 1/b} \} + \cdots \right]$$

(7-45)

where b and c are given by (7-24) and (7-33), respectively. We note here that the first term on the R. H. S. of (7-45) expresses the reciprocal of the Brooks-Herring relaxation time, (7-23).

It follows from (7-23) and (7-45) that the ratio of τ_i and τ_i^{B-H} is:

$$\frac{\tau_i}{\tau_i^{B-H}} = 1 - 4(\beta_{\underset{\sim}{k}}/b)\{\ln(1+b) - (1+b/2)b/(1+b)\}/\{\ln(1+b) - b/(1+b)\} + \cdots$$

(7-46)

We can see from (7-46) that the relaxation time due to the oscillating ionized impurities is slightly greater than that due to the fixed impurities. Physcally this means that the acoustic phonons induced by oscillating ionized impurities carry away the recoil momentum slightly less effectively. For example when $E_{\underset{\sim}{k}} = E_D$, i.e., when b = 4, the ratio of τ_i and τ_i^{B-H} is $1 + 9.4 \times 10^{-6}$, and in this case there is about 0.001 % increase in the relaxation time.

(ii) High Temperatures ($N_{\underset{\sim}{q}} >> 1$)

For high temperatures, from (7-42) and (7-44) we have the reciprocal of relaxation time for the Mossbauer type ionized impurity scattering as:

$$\frac{1}{\tau_i} = \frac{\pi Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2 (2m^*)^{\frac{1}{2}} E_{\underset{\sim}{k}}^{3/2}} \left[\{ \ln(1+b) - \frac{b}{1+b} \} + 4 \frac{c}{b} \{ \ln(1+b) - \frac{1 + b/2}{1 + 1/b} \} + \cdots \right] \tag{7-47}$$

where b and c are given be (7-24) and (7-40), respectively.
From (7-23) and (7-47), the ratio of τ_i and τ_i^{B-H} is:

$$\frac{\tau_i}{\tau_i^{B-H}} = 1 - 4(\beta'_{\underset{\sim}{k}}/b)\{\ln(1+b) - (1+b/2)b/(1+b)\}/\{\ln(1+b) - b/(1+b)\} + \cdots \tag{7-48}$$

where $\beta'_{\underset{\sim}{k}}$ and b are given by (7-40) and (7-24), respectively.

We now note that, since $\beta'_{\underset{\sim}{k}} > \beta_{\underset{\sim}{k}}$, τ_i at high temperatures may be somewhat greater than τ_i at low temperatures. Physically this means that the acoustic phonons induced by oscillating ionized impurities are more active at high temperatures than at low so that these acoustic phonons carry away the recoil momentum slightly less effectively at high temperatures than at low.

For example when $E_k = E_D$, i.e., when b = 4, the ratio of τ_i and τ_i^{B-H} is $1 + 9.4 \times 10^{-5}$, and in this case there is about 0.01 % increase in the relaxation time.

We conclude from these results obtained in (i) and (ii) that, even under these conditions of fairly hot electrons, the relaxation time-increase is only about 0.001 ~ 0.01 %. Our model, taking account of the impurity oscillation frequency common to lattice, does not modify the Brooks-Herring result appreciably.

PART III

8. Matrix Element for Inelastic Scattering

In Part II we considered the elastic scattering processes (i.e., the lattice state is unchanged), taking account of all the terms in the expansion of the exponential in powers of $\underset{\sim}{n}$. In this part, we shall consider only first-order processes for inelastic scattering.

From (5-2:C), the matrix element for the inelastic scattering is :

$$\langle \underset{\sim}{n}'\underset{\sim}{k}'|H_{int}|\underset{\sim}{n}\ \underset{\sim}{k}\rangle = \langle x_{\underset{\sim}{n}'}| \int_{\underset{\sim}{r}} \frac{-Ze^2\ e^{-k_D|\underset{\sim}{r}-\underset{\sim}{R}_i-\underset{\sim}{n}|}\ e^{i(\underset{\sim}{k}-\underset{\sim}{k}')\cdot\underset{\sim}{r}}}{\varepsilon_o V_o|\underset{\sim}{r}-\underset{\sim}{R}_i-\underset{\sim}{n}|} d\underset{\sim}{r}^3 |x_{\underset{\sim}{n}}\rangle \tag{8-1}$$

where $|\underset{\sim}{n}\underset{\sim}{k}\rangle$ is the state vector of the unperturbed Hamiltonian; $H_{lattice} + H_{electron}$, and is given by (6-2), the states $|\underset{\sim}{n}\rangle$ for the lattice and $|\underset{\sim}{k}\rangle$ for the conduction electron are given by (6-2:a) and (6-2:b), respectively. (8-1) shows that a lattice state goes from $\underset{\sim}{n}$ to $\underset{\sim}{n}'$ and a conduction electron goes from $\underset{\sim}{k}$ to $\underset{\sim}{k}'$, respectively, due to the interaction potential caused by the i^{th} ionized oscillating impurity.

As in Part II, letting $\underset{\sim}{\rho}=\underset{\sim}{r}-\underset{\sim}{R}_i-\underset{\sim}{n}$ and $\underset{\sim}{K}=\underset{\sim}{k}-\underset{\sim}{k}'$, (8-1) becomes :

$$\langle \underset{\sim}{n}'\underset{\sim}{k}'|H_{int}|\underset{\sim}{n}\underset{\sim}{k}\rangle = -\frac{4\pi\ Ze^2}{\varepsilon_o V_o(k^2+k_D^2)} e^{i\underset{\sim}{K}\cdot\underset{\sim}{R}_i}\left[\langle x_{\underset{\sim}{n}'}|e^{i\underset{\sim}{K}\cdot\underset{\sim}{n}}|x_{\underset{\sim}{n}}\rangle\right] \tag{8-2}$$

The exponential, $\exp(i\underset{\sim}{K}\cdot\underset{\sim}{r})$, may be expanded in power series with respect to $\underset{\sim}{r}$, and the last factor in (8-2) is reduced to:

$$\langle x_{\underset{\sim}{r}'}|e^{i\underset{\sim}{K}\cdot\underset{\sim}{r}}|x_{\underset{\sim}{r}}\rangle = \delta(\underset{\sim}{r}', \underset{\sim}{r}) + i\langle\underset{\sim}{r}'|\underset{\sim}{K}\cdot\underset{\sim}{r}|\underset{\sim}{r}\rangle + \cdots\cdots \qquad (8\text{-}3)$$

The first term on the R.H.S. of (8-3) corresponds to the elastic part while the second term corresponds to the first-order (one-phonon) processes for inelastic scattering, which is our main interest here. We may neglect the one-phonon processes arising from the higher order terms which are much smaller than the first-order term in $\underset{\sim}{r}$.

From (6-6), the second term in (8-3) is:

$$\begin{aligned}\langle\underset{\sim}{r}'|\underset{\sim}{K}\cdot\underset{\sim}{r}|\underset{\sim}{r}\rangle &= \sum_{\underset{\sim}{q}}\langle\underset{\sim}{r}'|W_{\underset{\sim}{q}}(B_{\underset{\sim}{q}}e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i} + B^{+}_{\underset{\sim}{q}}e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i})|\underset{\sim}{r}\rangle \\ &= \sum_{\underset{\sim}{q}} W_{\underset{\sim}{q}}\left\{e^{i\underset{\sim}{q}\cdot\underset{\sim}{R}_i}\, N^{\frac{1}{2}}_{\underset{\sim}{q}}\delta(N'_{\underset{\sim}{q}}, N_{\underset{\sim}{q}}-1) + e^{-i\underset{\sim}{q}\cdot\underset{\sim}{R}_i}(N_{\underset{\sim}{q}}+1)^{\frac{1}{2}}\delta(N'_{\underset{\sim}{q}}, N_{\underset{\sim}{q}}+1)\right\}\end{aligned} \qquad (8\text{-}4)$$

where $W_{\underset{\sim}{q}}$ is given by (6-8) and use has been made of (4-48) and (4-49).

From (8-2) and (8-4), the matrix elements of the first-order processes are reduced to:

$$\langle N_{\underset{\sim}{q}}-1, \underset{\sim}{k}'|H_{int}|N_{\underset{\sim}{q}}, \underset{\sim}{k}\rangle = -\,i\,\frac{4\pi Ze^2}{\varepsilon_o V_o(K^2+k_D^2)}\,W_{\underset{\sim}{q}}N^{\frac{1}{2}}_{\underset{\sim}{q}}\,e^{i(\underset{\sim}{K}+\underset{\sim}{q})\cdot\underset{\sim}{R}_i} \qquad (8\text{-}5\text{:a})$$

$$\langle N_{\underset{\sim}{q}}+1, \underset{\sim}{k}'|H_{int}|N_{\underset{\sim}{q}}, \underset{\sim}{k}\rangle = -\,i\,\frac{4\pi Ze^2}{\varepsilon_o V_o(K^2+k_D^2)}\,W_{\underset{\sim}{q}}(N_{\underset{\sim}{q}}+1)^{\frac{1}{2}}\,e^{i(\underset{\sim}{K}-\underset{\sim}{q})\cdot\underset{\sim}{R}_i} \qquad (8\text{-}5\text{:b})$$

where (8-5:a) and (8-5:b) correspond to the phonon absorption and the phonon emission processes, respectively. This interaction changes the state of the semiconductor by scattering the conduction electron from $\underset{\sim}{k}$ to $\underset{\sim}{k}'$ and either absorbing or emitting a phonon with mode $\underset{\sim}{q}$. Hence we can write:

$$\underset{\sim}{k}' - \underset{\sim}{k} \mp \underset{\sim}{q} = 0 \qquad (8\text{-}6)$$

8-1 Transition Probability

From (8-5:a,b), we have the squares of the matrix element for a phonon absorption and emission as:

$$\left| \langle N_{\underset{\sim}{q}}-1, \underset{\sim}{k}' | H_{int} | N_{\underset{\sim}{q}}, \underset{\sim}{k} \rangle \right|^2 = \frac{16\pi^2 Z^2 e^4}{\varepsilon_o^2 V_o^2 (K^2 + k_D^2)^2} W_{\underset{\sim}{q}}^2 N_{\underset{\sim}{q}} \qquad (8\text{-}7:a)$$

and

$$\left| \langle N_{\underset{\sim}{q}}+1, \underset{\sim}{k}' | H_{int} | N_{\underset{\sim}{q}}, \underset{\sim}{k} \rangle \right|^2 = \frac{16\pi^2 Z^2 e^4}{\varepsilon_o^2 V_o^2 (K^2 + k_D^2)^2} W_{\underset{\sim}{q}}^2 (N_{\underset{\sim}{q}}+1) \qquad (8\text{-}7:b)$$

respectively. Substituting (8-7:a) and (8-7:b) into (7-1), the corresponding Born approximation for the transition probability is:

$$P_{\underset{\sim}{k} \to \underset{\sim}{k}'} = \frac{2\pi}{\hbar} \frac{16\pi^2 Z^2 e^4}{\varepsilon_o^2 V_o^2 (K^2 + k_D^2)^2} W_{\underset{\sim}{q}}^2 N_{\underset{\sim}{q}} \delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} - \hbar\omega_q) \qquad (8\text{-}8:a)$$

when a phonon with mode $\underset{\sim}{q}$ is absorbed and

$$P_{\underset{\sim}{k}\to\underset{\sim}{k}'} = \frac{2\pi}{\hbar}\frac{16\,\pi^2 Z^2 e^4}{\varepsilon_o^2 V_o^2 (K^2 + k_D^2)^2} W_{\underset{\sim}{q}}^2 (N_{\underset{\sim}{q}}+1)\,\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} + \hbar\omega_q) \qquad (8\text{-}8\text{:b})$$

when a phonon with mode $\underset{\sim}{q}$ is emitted. Collecting the results (8-8:a,b), the transition probability rate for all phonon modes $\underset{\sim}{q}$ is:

$$P_{n\underset{\sim}{k}\to n\underset{\sim}{k}'} = \frac{2\pi}{\hbar}\sum_{\underset{\sim}{q}}\frac{16\,\pi^2 Z^2 e^4}{\varepsilon_o^2 V_o^2 (K^2 + k_D^2)^2} W_{\underset{\sim}{q}}^2 \Big\{ N_{\underset{\sim}{q}}\,\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} - \hbar\omega_q)$$

$$+ (N_{\underset{\sim}{q}}+1)\,\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} + \hbar\omega_q)\Big\} \qquad (8\text{-}9)$$

where δ-function ensures the energy conservation; a conduction electron in state $\underset{\sim}{k}$ is scattered onto one of two surfaces defined by the energy conservation relation $E_{\underset{\sim}{k}'} = E_{\underset{\sim}{k}} \pm \hbar\omega_q$. Since each scattering event of a conduction electron by impurity centres is assumed to be independent, we can sum (8-9) over all impurities, $N_D^{(+)}$, to give the total transition probability rate:

$$P^T_{n\underset{\sim}{k}\to n'\underset{\sim}{k}'} = \sum_{i=1}^{N_D^{(+)}} P_{n\underset{\sim}{k}\to n'\underset{\sim}{k}'} = \frac{32\,\pi^3 Z^2 e^4 n_D^{(+)}}{\hbar\,\varepsilon_o^2 V_o}\sum_{\underset{\sim}{q}}\frac{W_{\underset{\sim}{q}}^2}{(K^2 + k_D^2)^2}\Big\{ N_{\underset{\sim}{q}}\,\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} - \hbar\omega_q)$$

$$+ (N_{\underset{\sim}{q}}+1)\,\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} + \hbar\omega_q)\Big\}$$

$$= P^{A}(\underset{\sim}{k},\ \underset{\sim}{k}' = \underset{\sim}{k} + \underset{\sim}{q}) + P^{E}(\underset{\sim}{k},\ \underset{\sim}{k}' = \underset{\sim}{k} - \underset{\sim}{q}) \qquad (8\text{-}10)$$

where $n_D^{(+)} = N_D^{(+)}/V_o$ is the impurity density and

$$P^{A}(\underset{\sim}{k},\underset{\sim}{k}') = \frac{32\,\pi^3 Z^2 e^4 n_D^{(+)}}{\hbar\,\varepsilon_o^2\,V_o} \sum_{\underset{\sim}{q}} \frac{W_{\underset{\sim}{q}}^2}{(\,K^2 + k_D^2\,)^2}\, N_{\underset{\sim}{q}}\,\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} - \hbar\omega_q)$$

and (8-10:a)

$$P^{E}(\underset{\sim}{k},\underset{\sim}{k}') = \frac{32\,\pi^3 Z^2 e^4 n_D^{(+)}}{\hbar\,\varepsilon_o^2\,V_o} \sum_{\underset{\sim}{q}} \frac{W_{\underset{\sim}{q}}^2}{(\,K^2 + k_D^2\,)^2}\, (N_{\underset{\sim}{q}} + 1\,)\,\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} + \hbar\omega_q)$$

(8-10:b)

are the transition probability rate for phonon absorption and the phonon emission processes, respectively.

9. Collision Term

Using the transition probability,(8-10), that a conduction electron in a state $\underset{\sim}{k}$ makes a transition to another state $\underset{\sim}{k}'$ by either absorbing or emitting a phonon and taking into account the property of micro-reversibility and of the probability of electron occupations, $f(\underset{\sim}{k})\{1-f(\underset{\sim}{k}')\}$, i.e., the probability that the initial state $\underset{\sim}{k}$ is occupied and the final state $\underset{\sim}{k}'$ is unoccupied, the collision term in the Boltzmann equation is:

$$\left(\frac{\partial f(\underset{\sim}{k})}{\partial t}\right)_{\text{collision}} = \sum_{\underset{\sim}{k}'} \left[P^T(\underset{\sim}{k}',\underset{\sim}{k}) f(\underset{\sim}{k}')(1-f(\underset{\sim}{k})) - P^T(\underset{\sim}{k},\underset{\sim}{k}') f(\underset{\sim}{k})(1-f(\underset{\sim}{k}')) \right]$$

$$= \sum_{\underset{\sim}{k}'} \Big[P^E(\underset{\sim}{k}',\underset{\sim}{k}) f(\underset{\sim}{k}')(1-f(\underset{\sim}{k})) + P^A(\underset{\sim}{k}',\underset{\sim}{k}) f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))$$

$$- P^E(\underset{\sim}{k},\underset{\sim}{k}') f(\underset{\sim}{k})(1-f(\underset{\sim}{k}')) - P^A(\underset{\sim}{k},\underset{\sim}{k}') f(\underset{\sim}{k})(1-f(\underset{\sim}{k}')) \Big] \qquad (9\text{-}1)$$

where the first, second, third and fourth term of (9-1) correspond to the following diagrams respectively.

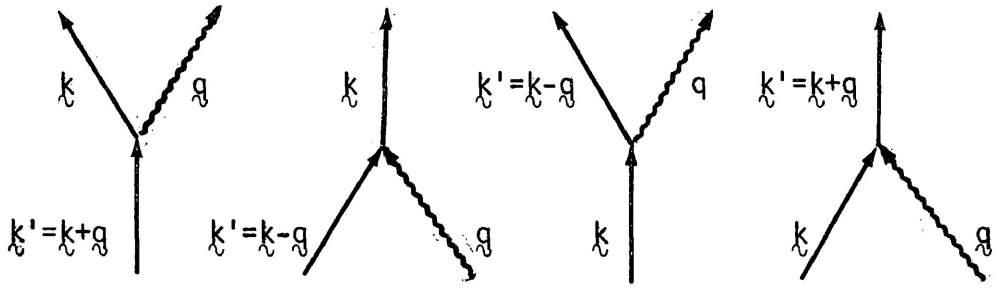

Fig. I Diagrams of Scattering Processes

Substituting (8-10:a,b) into (9-1), we obtain:

$$\left(\frac{\partial f(\underset{\sim}{k})}{\partial t}\right)_{\text{collision}} = \frac{16\,\pi^3 Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2\,\rho_o\,S_o\,V_o^2} \sum_{\underset{\sim}{k}'} \sum_{\underset{\sim}{q}} \frac{q}{(q^2 + k_D^2)^2} \Big[(N_{\underset{\sim}{q}}+1) f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))$$

$$\times \delta(E_{\underset{\sim}{k}} - E_{\underset{\sim}{k}'} + \hbar\omega_{\underset{\sim}{q}}) + N_{\underset{\sim}{q}} f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))\delta(E_{\underset{\sim}{k}} - E_{\underset{\sim}{k}'} - \hbar\omega_{\underset{\sim}{q}}) - (N_{\underset{\sim}{q}}+1) f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))$$

$$\times \delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q) - N_{\underset{\sim}{q}} f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)\Big] \qquad (9\text{-}2)$$

where use has been made of (6-8), noting $\underset{\sim}{K} = \underset{\sim}{k} - \underset{\sim}{k}' = \pm\underset{\sim}{q}$.

Introducing the density of lattice states and the density of electron states given by (7-26) with (7-27) and by (7-15) respectively, we can replace the sum over all lattice modes, $\underset{\sim}{q}$, and the final electron states, $\underset{\sim}{k}'$, by integrals. Thus (9-2) becomes:

$$\left(\frac{\partial f(\underset{\sim}{k})}{\partial t}\right)_{\text{collision}} = \frac{3\, Z^2 e^4 n_D^{(+)}}{4\,\pi^3 \varepsilon_o^2 \rho_o S_o} \iint_{\underset{\sim}{k}'\,\underset{\sim}{q}} \frac{q}{(q^2+k_D^2)^2} \Big[(N_{\underset{\sim}{q}}+1) f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))$$

$$\times \delta(E_{\underset{\sim}{k}}-E_{\underset{\sim}{k}'}+\hbar\omega_q) + N_{\underset{\sim}{q}} f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))\delta(E_{\underset{\sim}{k}}-E_{\underset{\sim}{k}'}-\hbar\omega_q) - (N_{\underset{\sim}{q}}+1) f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))$$

$$\times \delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q) - N_{\underset{\sim}{q}} f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)\Big] d\underset{\sim}{k}'^3 d\underset{\sim}{q}^3$$

(9-3)

The first two terms in (9-3) give the number of conduction electrons scattered into the state $\underset{\sim}{k}$ and the last two in (9-3) give the number of conduction electrons scattered out of the state $\underset{\sim}{k}$ per unit time, either by emission or absorption of an acoustic phonon.

The expression of (9-3) may be simplified if it is assumed that the phonon number, $N_{\underset{\sim}{q}}$, is determined by the equilibrium distribution function (7-31). However, we note here that the use of (7-31) in (9-3) is not always justified. But it will be satisfactory whenever the relaxation processes which establish equilibrium of the phonon distribution are rapid compared to that which operate to return the electronic distribution to equilibrium. In this case, we proceed under the assumption that (7-31) may be valid to use.

9-1 Thermal Equilibrium Situation

If the system is in equilibrium, the collision term, (9-3), is zero. This is easily proved (see Appendix B) by replacing $N_{\underset{\sim}{q}}$ for phonons by (7-31) and $f(\underset{\sim}{k})$ for electrons by:

$$f^{\circ}(k) = \left[e^{(E_{\underset{\sim}{k}}-\mu)/k_B T_e} + 1 \right]^{-1} \qquad (9\text{-}4)$$

for their equilibrium distribution functions, respectively.

At the equilibrium, the following useful relations hold:

$$\{(N_{\underset{\sim}{q}}+1)f^{\circ}(\underset{\sim}{k}')(1-f^{\circ}(\underset{\sim}{k}))\}\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q) = \{N_{\underset{\sim}{q}}f^{\circ}(\underset{\sim}{k})(1-f^{\circ}(\underset{\sim}{k}'))\}\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)$$

(9-5:a)

$$\{(N_{\underset{\sim}{q}}+1)f^{\circ}(\underset{\sim}{k})(1-f^{\circ}(\underset{\sim}{k}'))\}\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q) = \{N_{\underset{\sim}{q}}f^{\circ}(\underset{\sim}{k}')(1-f^{\circ}(\underset{\sim}{k}))\}\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)$$

(9-5:b)

10. Derivation of Linearized Boltzmann Equation

When the system is in a uniform weak electric field $\underset{\sim}{E}$, the Boltzmann equation can be written as:

$$\frac{e\,\underset{\sim}{E}}{\hbar}\cdot\frac{\partial f(\underset{\sim}{k})}{\partial \underset{\sim}{k}} = \left(\frac{\partial f(\underset{\sim}{k})}{\partial t}\right)_{\text{collision}} \tag{10-1}$$

If we assume that the collision term can be taken to be of the form (the relaxation time approximation):

$$\left(\frac{\partial f(\underset{\sim}{k})}{\partial t}\right)_{\text{collision}} = -\frac{f(\underset{\sim}{k}) - f^{o}(\underset{\sim}{k})}{\tau(\underset{\sim}{k})} \tag{10-2}$$

then we may solve (10-1) easily. (10-2) implies that any change in $f(\underset{\sim}{k})$ from its equilibrium value will relax exponentially with a time constant τ towards the equilibrium value $f^{o}(\underset{\sim}{k})$. We note that a thermal gradient is assumed to be absent so that the distribution $f(\underset{\sim}{k})$ is only a function of $\underset{\sim}{k}$ and t. Therefore from (10-1) and (10-2), we have, within a first power of $\underset{\sim}{E}$,

$$f(\underset{\sim}{k}) = f^{o}(\underset{\sim}{k}) - \tau\frac{e\,\underset{\sim}{E}}{\hbar}\cdot\frac{\partial f^{o}(\underset{\sim}{k})}{\partial \underset{\sim}{k}} \tag{10-3}$$

where $f^{\circ}(\underset{\sim}{k})$ is the equilibrium distribution function and is given by (9-4).

Since f° depends on $\underset{\sim}{k}$ through the electron energy $E_{\underset{\sim}{k}}$ ($= \hbar^2 k^2/2m^*$ based on the simple effective mass model), we have:

$$\frac{\partial f^{\circ}(\underset{\sim}{k})}{\partial \underset{\sim}{k}} = \frac{\partial f^{\circ}}{\partial E_{\underset{\sim}{k}}} \cdot \frac{\partial E_{\underset{\sim}{k}}}{\partial \underset{\sim}{k}} = \frac{\hbar^2 \underset{\sim}{k}}{m^*} \cdot \frac{\partial f^{\circ}}{\partial E_{\underset{\sim}{k}}} \qquad (10\text{-}4)$$

where:

$$\frac{\partial f^{\circ}}{\partial E_{\underset{\sim}{k}}} = - \frac{\beta\, e^{(E_{\underset{\sim}{k}}-\mu)}}{\left(e^{\beta(E_{\underset{\sim}{k}}-\mu)} + 1 \right)^2} = - \beta f^{\circ}(\underset{\sim}{k})(1-f^{\circ}(\underset{\sim}{k})) \qquad (10\text{-}5)$$

and $\beta = (k_B T_e)^{-1}$. Hence we can write (10-3) as:

$$f(\underset{\sim}{k}) = f^{\circ}(\underset{\sim}{k}) - \Phi(\underset{\sim}{k}) \cdot \frac{\partial f^{\circ}}{\partial E_{\underset{\sim}{k}}} \qquad (10\text{-}6)$$

where: $\Phi(\underset{\sim}{k}) \equiv \frac{\tau e \hbar}{m^*} (\underset{\sim}{k} \cdot \underset{\sim}{E})$ (10-7)

$\Phi(\underset{\sim}{k})$ is defined by (10-7) and is now the unknown function and assumed to be small. Substituting (10-6) into (9-3), keeping only terms with the first power of Φ (since we are considering the terms with the first power of $\underset{\sim}{E}$) and using (9-5:a,b), after some manipulation (see Appendix C),

the collision term (9-3) becomes:

$$\left(\frac{\partial f(\underset{\sim}{k})}{\partial t}\right)_{\text{collision}} = \frac{3Z^2e^4n_D^{(+)}\beta}{4\pi^3\varepsilon_o^2\rho_oS_o}\iint\frac{q}{(q^2+k_D^2)^2}N_{\underset{\sim}{q}}\Big[f^o(\underset{\sim}{k})(1-f^o(\underset{\sim}{k}'))$$

$$\times\,\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q) + f^o(\underset{\sim}{k}')(1-f^o(\underset{\sim}{k}))\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)\Big]\Big[\Phi(\underset{\sim}{k}') - \Phi(\underset{\sim}{k})\Big]d\underset{\sim}{k}'^3d\underset{\sim}{q}^3$$

(10-8)

where we have made use of (10-5), and $\underset{\sim}{k}' = \underset{\sim}{k} \pm \underset{\sim}{q}$ for either a phonon absorption (+) or phonon emission (-) processes.

From (10-1), (10-3) and (10-8), the linearized Boltzmann equation is:

$$\frac{3Z^2e^4n_D^{(+)}\beta}{4\pi^3\varepsilon_o^2\rho_oS_o}\iint\frac{q}{(q^2+k_D^2)^2}N_{\underset{\sim}{q}}\Big[\Phi(\underset{\sim}{k}') - \Phi(\underset{\sim}{k})\Big]\,\Psi\,d\underset{\sim}{k}'^3d\underset{\sim}{q}^3 = \frac{e\underset{\sim}{E}}{\hbar}\cdot\frac{\partial f^o(\underset{\sim}{k})}{\partial\underset{\sim}{k}}$$

(10-9)

where: $\Psi \equiv f^o(\underset{\sim}{k})[1-f^o(\underset{\sim}{k}')]\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q) + f^o(\underset{\sim}{k}')[1-f^o(\underset{\sim}{k}')]\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)$

(10-10)

Note that $\Phi(\underset{\sim}{k})$ is derived under the assumption that the energy $E_{\underset{\sim}{k}}$ is a quadratic function of $\underset{\sim}{k}$. If we assume $\underset{\sim}{E} = (0, 0, E_z)$, (10-9) becomes:

$$\frac{3Z^2e^4n_D^{(+)}\hbar\beta}{4\pi^3\varepsilon_o\rho_o S_o}\iint\frac{q}{(q^2+k_D^2)^2}N_{\underset{\sim}{q}}\left[k'_z\,\tau(\underset{\sim}{k}') - k_z\tau(\underset{\sim}{k})\right]\Psi\, d\underset{\sim}{k}'^3 d\underset{\sim}{q}^3$$

$$= \frac{m^*}{\hbar}\cdot\frac{\partial f^o(\underset{\sim}{k})}{\partial k_z} \qquad (10\text{-}11)$$

where Ψ is given by (10-10). (10-11) is the basic equation to determine relaxation time τ.

11. Relaxation Time for Momentum Transfer (Inelastic Case)

For lightly doped, nondegenerate semiconductors we can use the Boltzmann distribution function for conduction electrons;

$$f^o(\underset{\sim}{k}) = e^{-(E_{\underset{\sim}{k}}-\mu)/k_BT_e} \qquad (11\text{-}1)$$

in stead of the Fermi-Dirac distribution function (9-4). Hence we can replace the square brackets in (10-10) by unity. The basic equation for nondegenerate semiconductors may be written as:

$$\frac{3Z^2e^4n_D^{(+)}\hbar\beta}{4\pi^3\varepsilon_o^2\rho_o S_o}\iint\frac{q}{(q^2+k_D^2)^2}N_q\left[k_z'\tau(\underset{\sim}{k}') - k_z\tau(\underset{\sim}{k})\right]\left[f^o(\underset{\sim}{k})\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)\right.$$

$$\left. + f^o(\underset{\sim}{k}')\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)\right]d\underset{\sim}{k}'^3d\underset{\sim}{q}^3 = \frac{m^*}{\hbar}\cdot\frac{\partial f^o(\underset{\sim}{k})}{\partial k_z} \qquad (11\text{-}2)$$

We first integrate (11-2) over $\underset{\sim}{k}'$. Noting $f^o(\underset{\sim}{k}) = f^o(E_{\underset{\sim}{k}})$ and that $k^2dk = \{(2m^*)^{3/2}/2\hbar^3\}E_{\underset{\sim}{k}}^{\frac{1}{2}}dE_{\underset{\sim}{k}}$, and since $E_{\underset{\sim}{k}} = \hbar^2\underset{\sim}{k}^2/2m^*$, we have:

$$\int\left[k_z'\tau(\underset{\sim}{k}') - k_z\tau(\underset{\sim}{k})\right]\left[f^o(\underset{\sim}{k})\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q) + f^o(\underset{\sim}{k}')\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)\right]d\underset{\sim}{k}'^3$$

$$= 2\pi\iint\left[(k'\cos\theta_{\underset{\sim}{k}'})\tau(\underset{\sim}{k}') - k_z\tau(\underset{\sim}{k})\right]\left[f^o(\underset{\sim}{k})\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q) + f^o(\underset{\sim}{k}')\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)\right]$$

$$\times k'^2\sin\theta_{\underset{\sim}{k}'}d\theta_{\underset{\sim}{k}'}dk'$$

$$= -\frac{2\pi k_z(2m^*)^{3/2}\tau(\underset{\sim}{k})}{\hbar^3}\left[f^o(E_{\underset{\sim}{k}})\int E_{\underset{\sim}{k}'}^{\frac{1}{2}}\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)dE_{\underset{\sim}{k}'} + \int E_{\underset{\sim}{k}'}^{\frac{1}{2}}f^o(E_{\underset{\sim}{k}'})\right.$$

$$\left.\times\,\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)dE_{\underset{\sim}{k}'}\right]$$

$$= -\frac{2\pi k_z(2m^*)^{3/2}\tau(\underset{\sim}{k})}{\hbar^3}\left[(E_{\underset{\sim}{k}}+\hbar\omega_q)^{\frac{1}{2}}f^o(E_{\underset{\sim}{k}}) + (E_{\underset{\sim}{k}}-\hbar\omega_q)^{\frac{1}{2}}f^o(E_{\underset{\sim}{k}}-\hbar\omega_q)\right]$$

(11-3)

From (11-2) and (11-3) we have the reciprocal of relaxation time for momentum transfer as:

$$\frac{1}{\tau_i} = -\frac{3Z^2e^4(2m^*)^{\frac{1}{2}}n_D^{(+)}k_z}{\pi^2\varepsilon_o^2\rho_o S_o \hbar k_B T_e}\cdot\left(\frac{\partial f^o(E_{\underset{\sim}{k}})}{\partial k_z}\right)^{-1}\int\frac{q}{(q^2+k_D^2)^2}N_{\underset{\sim}{q}}$$

$$\times\left[(E_{\underset{\sim}{k}}+\hbar\omega_q)^{\frac{1}{2}}f^o(E_{\underset{\sim}{k}}) + (E_{\underset{\sim}{k}}-\hbar\omega_q)^{\frac{1}{2}}f^o(E_{\underset{\sim}{k}}-\hbar\omega_q)\right]d\underset{\sim}{q}^3 \qquad (11\text{-}4)$$

For semiconductor $E_{\underset{\sim}{k}}$ is of the order of thermal energy of a conduction electron; $E_{\underset{\sim}{k}} = 3k_BT_e/2$, and Max $\hbar\omega_q$ is of the order of $k_B\Theta = \hbar S_o q_{max}$, where Θ is the Debye temperature of the bulk material. If $T_e >> \Theta$, we can approximate:

$$(E_{\underset{\sim}{k}} \pm \hbar\omega_q)^{\frac{1}{2}} = E_{\underset{\sim}{k}}^{\frac{1}{2}}\left(1 \pm \tfrac{1}{2}\hbar\omega_q/E_{\underset{\sim}{k}} - \cdots\cdots\cdots\right) \qquad (11\text{-}5)$$

and noting $\hbar\omega_q = \hbar S_o q << k_BT_e$, we can write:

$$f^o(E_{\underset{\sim}{k}} - \hbar\omega_q) = e^{(E_{\underset{\sim}{k}}-\hbar\omega_q-\mu)/k_BT_e} = e^{-\hbar\omega_q/k_BT_e}\, f^o(E_{\underset{\sim}{k}}) \simeq f^o(E_{\underset{\sim}{k}}).$$

(11-6)

Thus:

$$\frac{\partial f^{\circ}(E_{\underset{\sim}{k}})}{\partial K_z} = \frac{\partial f^{\circ}(E_{\underset{\sim}{k}})}{\partial E_{\underset{\sim}{k}}} \cdot \frac{\partial E_{\underset{\sim}{k}}}{\partial k_z} = - \frac{\hbar^2 k_z}{m^* k_B T_e} f^{\circ}(E_{\underset{\sim}{k}}) \qquad (11\text{-}7)$$

where use has been made of (11-1) and $E_{\underset{\sim}{k}} = \hbar^2 \underset{\sim}{k}^2 / 2m^*$.

From (11-5), (11-6) and (11-7), (11-4) becomes:

$$\frac{1}{\tau_i} = \frac{3Z^2 e^4 (2m^*)^{3/2} n_D^{(+)}}{\pi^2 \varepsilon_o^2 \rho_o S_o \hbar^3} E_{\underset{\sim}{k}}^{\frac{1}{2}} \int \frac{q}{(q^2 + k_D^2)^2} N_{\underset{\sim}{q}} \, d\underset{\sim}{q}^3 \qquad (11\text{-}8)$$

where $N_{\underset{\sim}{q}}$ is defined by the Planck distribution function, (7-31), which follows:

$$N_{\underset{\sim}{q}} \simeq k_B T / \hbar S_o q \qquad (11\text{-}9)$$

for $k_B T \gg \hbar S_o q$. This high temperature approximation is valid for temperatures , $T \gtrsim 1\ ^{\circ}K$.

From (11-8) and (11-9), we have, after angular integrations;

$$\frac{1}{\tau_i} = \frac{12 Z^2 e^4 (2m^*)^{3/2} n_D^{(+)} k_B T E_{\underset{\sim}{k}}^{\frac{1}{2}}}{\pi \varepsilon_o^2 \rho_o S_o^2 \hbar^4} \int \frac{q^2}{(q^2 + k_D^2)^2} \, dq \qquad (11\text{-}10)$$

It is important to note that the integration is carried out over the whole range of values of q. We shall determine the limits of this range.

If the energy of a conduction electron is $E_{\underset{\sim}{k}} = \hbar^2 \underset{\sim}{k}^2/2m^*$ and the frequency of the longitudinal acoustical waves is $\omega_q = S_o q$, where S_o is the speed of these waves, it follows from the law of energy conservation (recall that δ-function ensures the energy conservation of the system) that:

$$E_{\underset{\sim}{k}'} = E_{\underset{\sim}{k}} \pm \hbar\omega_q \quad \text{i.e.,} \quad \frac{\hbar^2(\underset{\sim}{k} \pm \underset{\sim}{q})^2}{2m^*} = \frac{\hbar^2 \underset{\sim}{k}^2}{2m^*} \pm \hbar S_o q \qquad (11\text{-}11)$$

The upper sign represents the absorption of an acoustic phonon and the lower sign the emission of an acoustic phonon. Therefore,

$$q = \mp 2k \cos\theta \pm 2m^* S_o/\hbar \qquad (11\text{-}12)$$

where θ is the angle between the directions of the vectors $\underset{\sim}{k}$ and $\underset{\sim}{q}$. We shall find the second term in (11-12), dividing it by k,

$$2m^* S_o/\hbar k = 2m^* S_o/p = 2m^* S_o/\sqrt{3m^* k_B T_e} = 2\sqrt{T/T_e} \qquad (11\text{-}13)$$

where $T = m^* S_o^2/3k_B$, and k_B is the Boltzmann's constant. Since conduction electrons are distributed in accordance with Boltzmann's law, we can assume that the average value of p is $\sqrt{3m^* k_B T_e}$. If $S_o = 10^5$ Cm/sec and $m^* = 0.5 \times 10^{-27}$g, we find $T < 1\ ^\circ K$. At all temperatures $T_e >> 1\ ^\circ K$, we can neglect the second term in (11-12) and, therfore,

$$q = \mp 2k \cos\theta \qquad (11\text{-}14)$$

which shows that the range of integration with respect to q extends from q = 0 to q = 2k. Neglecting the term $2m^*S_o/\hbar$ is equivalent to neglecting the second term in (11-11), i.e., equivalent to neglecting the term describing the inelasticity of electron-phonon collisions. But an electron in a state $\underset{\sim}{k}$ is actually not scattered onto a surface of constant energy $E_{\underset{\sim}{k}'} = E_{\underset{\sim}{k}}$ but onto one of two surfaces slightly displaced in energy, $\hbar\omega_q$, from it.

Since the average value of k for electron at 300°K is about $10^7 Cm^{-1}$, and according to the Debye theory the value of q_{max} is, from (7-28), $10^8 Cm^{-1}$, it follows that $2k < q_{max}$. We therefore take 2k for the upper limit of the integral in (11-10) for semiconductors. Hence the integral in (11-10) becomes:

$$\int_0^{2k} \frac{q^2}{(q^2 + k_D^2)^2}\, dq = \left[-\frac{q}{2(q^2+k_D^2)} + \frac{1}{2k_D} \tan^{-1}(q/k_D) \right]_0^{2k}$$

$$= -\frac{k}{4k^2 + k_D^2} + \frac{1}{2k_D} \tan^{-1}(2k/k_D)$$

$$\equiv F(2k/k_D) \qquad (11\text{-}15)$$

Hence from (11-10) and (11-15), the reciprocal of relaxation time due to ionized oscillating impurities is:

$$\frac{1}{\tau_i} = \frac{12Z^2e^4(2m^*)^{3/2}n_D^{(+)}k_BT\ E_{\underset{\sim}{k}}^{\frac{1}{2}}}{\pi\ \varepsilon_o^2\ \rho_o\ S_o^2\ \hbar^4} F(2k/k_D)$$

$$= \frac{3}{2\pi} \cdot \frac{(2m^*)^{3/2}}{\hbar^4} \cdot \frac{k_BT}{\rho_o S_o^2} \cdot \frac{4Z^2e^4n_D^{(+)}}{\varepsilon_o^2\ k_D} E_{\underset{\sim}{k}}^{\frac{1}{2}}\ G(2k/k_D) \qquad (11\text{-}16)$$

where use has been made of (5-3) in which n_o is replaced by $Zn_D^{(+)}$. Here $G(k/2k_D)$ is given by:

$$G(2k/k_D) = \tan^{-1}(2k/k_D) - \frac{2k/k_D}{1 + (2k/k_D)^2} \qquad (11\text{-}17)$$

Note that (11-16) is valid except for extremely low temperatures.

(i) Fairly Low Temperatures and High Impurity Concentration

In this case the condition, $2k \ll k_D$, is satisfied, so that we can expand the terms in (11-17) to give $G(2k/k_D)$ as:

$$G(2k/k_D) = 2k/k_D - (2k/k_D)^3/3 + \cdots\cdots - \{1-(2k/k_D)^2\}2k/k_D + \cdots$$

$$\doteq \frac{2}{3}\left(\frac{2k}{k_D}\right)^3 \qquad (11\text{-}18)$$

We, therefore, have the reciprocal of relaxation time as:

$$\frac{1}{\tau_i} = \frac{8}{9\pi^3}\cdot\frac{(2m^*)^3}{\hbar^7}\cdot\frac{k_B T}{\rho_o S_o^2\, n_D^{(+)}}\, E_{\underset{\sim}{k}}^4$$

$$= \frac{9}{2\pi^3}\cdot\frac{(2m^*)^3\, k_B^5}{\hbar^7}\cdot\frac{T\, T_e^4}{\rho_o S_o^2\, n_D^{(+)}} \qquad (11\text{-}19)$$

where we have used (5-3) in which n_o is replaced by $Zn_D^{(+)}$ when all impurities are ionized, and $E_{\underset{\sim}{k}} = \hbar^2 \underset{\sim}{k}^2/2m^* = 3k_B T_e/2$.

(ii) High Temperatures and Low Impurity Concentration

In this case the condition, $2k \gg k_D$, is satisfied, so that (11-17) approximates to:

$$G(2k/k_D) \doteqdot \tan^{-1}(2k/k_D) \qquad (11\text{-}20)$$

We, therefore, have the reciprocal of relaxation time as:

$$\frac{1}{\tau_i} = \frac{6^{\frac{1}{2}}}{\pi^{3/2}}\cdot\frac{(2m^*)^{3/2}}{\hbar^4}\cdot\frac{(Ze^2)^{3/2}}{\varepsilon_o^{3/2}}\cdot\frac{k_B T}{\rho_o S_o^2}\, n_D^{(+)\frac{1}{2}}\, E_{\underset{\sim}{k}}\, \tan^{-1}\left[\left(\frac{4\varepsilon_o m^*}{3\pi Zn_D^{(+)}}\right)^{\frac{1}{2}}\frac{E_{\underset{\sim}{k}}}{e\hbar}\right]$$

$$= 3\left(\frac{3}{2}\right)^{\frac{1}{2}}\frac{(2m^*)^{3/2}}{\hbar^4}\cdot\frac{(Ze^2)^{3/2}}{\varepsilon_o^{3/2}}\cdot\frac{k_B^2}{\rho_o S_o^2}\, n_D^{(+)\frac{1}{2}}\, T\, T_e\, \tan^{-1}\left[\left(\frac{3\varepsilon_o m^*}{4\pi Zn_D^{(+)}}\right)^{\frac{1}{2}}\frac{k_B T_e}{e\hbar}\right]$$

(11-22)

where we have used (5-3) in which n_o is replaced by $Zn_D^{(+)}$ when all impurities are ionized, and $E_{\underset{\sim}{k}} = \hbar^2 \underset{\sim}{k}^2/2m^* = 3k_B T_e/2$.

12. Effective Relaxation Time (Mixed Scattering)

In real crystals, several scattering mechanisms usually act simultaneously. In fact, in every interpretation of the results obtained for a given transport phenomenon we are faced with the problem of the mixed scattering of conduction electrons; these scattering mechanisms are usually the scattering by ionized impurities and by acoustic phonons.

Applying the well-known addition rule to the reciprocals $1/\tau$:

$$\frac{1}{\tau_{eff}} = \sum_{\nu} \frac{1}{\tau_\nu} \tag{12-1}$$

we obtain the following expression for the simultaneous scattering by the acoustic phonons and oscillating ionized impurities:

$$\frac{1}{\tau_{eff}} = \frac{1}{\tau_p} + \frac{1}{\tau_i} = \frac{1}{\tau_p}\left(1 + \frac{\tau_p}{\tau_i}\right) \tag{12-2}$$

where τ_i is given by (11-16) and τ_p is the relaxaion time due to the ordinary electron-phonon scattering (see Appendix D for derivation) and is given by:

$$\frac{1}{\tau_p} = \frac{1}{2\pi} \cdot \frac{(2m^*)^{3/2}}{\hbar^4} \cdot \frac{k_B T}{\rho_o S_o^2} C^2 E_{\underset{\sim}{k}}^{\frac{1}{2}} \qquad (12\text{-}3)$$

where C is the deformation potential constant (the electron-phonon coupling constant) and $E_{\underset{\sim}{k}}$ is the average energy of a conduction electron ($E_{\underset{\sim}{k}} = \hbar^2 \underset{\sim}{k}^2/2m^* \equiv 3k_B T_e/2$). We note here that the acoustic phonon scattering is encountered in intrinsic semiconductors.

Since the temperature range valid for both τ_p and τ_i is the same ; i.e., $T > 1^oK$, we may find the effective relaxation time, (12-2), in extrinsic semiconductors.

12-1 Oscillating Ionized Impurity Effect

To calculate the effect of oscillating ionized impurities on τ_{eff}, we consider τ_p/τ_i. From (11-16) and (12-3),

$$\frac{\tau_p}{\tau_i} = \frac{12Z^2 e^4 n_D^{(+)}}{\varepsilon_o^2 C^2 k_D} G(2k/k_D) \qquad (12\text{-}4)$$

where $G(2k/k_D)$ is given by (11-17) and k_D by (5-3) in which n_o is replaced by $Zn_D^{(+)}$ when all impurities are ionized. Then k_D is called the screening wave number (the extrinsic Debye wave number).

Assuming $C \simeq 1.76 \times 10^{-11}$ erg, $m^* \simeq 2.004 \times 10^{-28}$ g, $\varepsilon_o \simeq 15.8$ and that the impurities are singly ionized (i.e., $Z = 1$), we have, from (5-3), (11-17), (12-4) and using $k = (3m^* k_B T_e)^{\frac{1}{2}}/\hbar$, for a thermal electron:

$$\frac{\tau_p}{\tau_i} \simeq 1.066 \times 10^{-4} \qquad \text{for } T_e = 300\ ^\circ K,\ n_D^{(+)} = 10^{17}\ Cm^{-3}$$

$$\frac{\tau_p}{\tau_i} \simeq 9.867 \times 10^{-4} \qquad \text{for } T_e = 300\ ^\circ K,\ n_D^{(+)} = 10^{21}\ Cm^{-3}$$

$$\frac{\tau_p}{\tau_i} \simeq 2.011 \times 10^{-4} \qquad \text{for } T_e = 10^3\ ^\circ K,\ n_D^{(+)} = 10^{17}\ Cm^{-3}$$

$$\frac{\tau_p}{\tau_i} \simeq 5.657 \times 10^{-3} \qquad \text{for } T_e = 10^3\ ^\circ K,\ n_D^{(+)} = 10^{21}\ Cm^{-3}$$

From the above results and (12-2), we have:

$$(\tau_{eff}-\tau_p)/\tau_p \times 100\ \% \simeq -0.01\ \% \text{ for } T_e = 300\ ^\circ K,\ n_D^{(+)} = 10^{17}\ Cm^{-3}$$

$$(\tau_{eff}-\tau_p)/\tau_p \times 100\ \% \simeq -0.10\ \% \text{ for } T_e = 300\ ^\circ K,\ n_D^{(+)} = 10^{21}\ Cm^{-3}$$

$$(\tau_{eff}-\tau_p)/\tau_p \times 100\ \% \simeq -0.02\ \% \text{ for } T_e = 10^3\ ^\circ K,\ n_D^{(+)} = 10^{17}\ Cm^{-3}$$

$$(\tau_{eff}-\tau_p)/\tau_p \times 100\ \% \simeq -0.56\ \% \text{ for } T_e = 10^3\ ^\circ K,\ n_D^{(+)} = 10^{21}\ Cm^{-3}$$

We conclude from these results that the oscillating ionized impurity effect is too small to be observable at temperatures $T_e > 1\ ^{\circ}K$, but we see that as temperature or impurity density is increased, oscillating impurity effect is slightly increased. Physically this means that as temperature is increased, electron-phonon scattering is more active, not only due to the oscillation of solvent atoms but also due to that of impurity atoms. Hence electron-phonon scattering through impurity oscillations should be taken into account. Since impurity atoms also oscillate like solvent atoms, as impurity densities are increased, electron-phonon scattering through the impurity oscillations contribute to the effective scattering mechanisms.

12-2 Oscillating Ionized Impurity Effect on the Deformation Potential (or the Electron-Phonon Coupling) Constant

Comparing (11-16) with (12-3), we have the effective deformation potential (or the effective electron-phonon coupling) constant, C_{eff}, as:

$$C_{eff} \simeq C\{\ 1 + \frac{6Z^2e^4n_D^{(+)}}{\varepsilon_o^2 k_D C^2} G(2k/k_D)\} \qquad (12\text{-}5)$$

where $G(2k/k_D)$ is given by (11-17).

We see from (12-5) that as $n_D^{(+)} \to 0$ or $k_D \to \infty$ (i.e., $T_e \to 0$), $C_{eff} \to C$, i.e., the effective deformation potential (electron-phonon) coupling constant, C_{eff}, goes to that for intrinsic semiconductors.

Using the results obtained in the previous section, we have $C_{eff} = C_{eff}(T_e, n_D^{(+)})$ as follows:

$$C_{eff}(300,10^{17}) \simeq (1 + 5.330 \times 10^{-5})C$$

$$C_{eff}(300,10^{21}) \simeq (1 + 4.934 \times 10^{-4})C$$

$$C_{eff}(10^3,10^{17}) \simeq (1 + 1.006 \times 10^{-4})C$$

$$C_{eff}(10^3,10^{21}) \simeq (1 + 2.829 \times 10^{-3})C$$

where the units of T_e and $n_D^{(+)}$ are $^\circ K$ and Cm^{-3}, respectively.

We conclude from the above results that the effective deformation potential energy is slightly increased at higher temperatures or higher impurity densities but these effects (due to the oscillating ionized impurities) are too small to be observable at the temperatures, $T_e \gtrsim 1\ ^\circ K$.

Conclusions

From the analysis and the computed results presented in the previous chapters, tentative conclusions are drawn as follows:

(i) The effect of the impurity oscillation tends to increase the effective deformation potential coupling constant, C_{eff}. In the case of high temperature apporoximation, such a change is still less than 1 % for most non-degenerate non-polar semiconductors.

(ii) This effect tends also to decrease the effective electron-phonon relaxation time since it is inversely proportional to C_{eff}^2. This implies that this effect tends to lower the electron mobility. However the lowering is small, and it would be less than 1 % even at temperatures up to the melting point and with impurity concentrations reaching the degenerate conditions.

(iii) These theoretical results are essentially the same as those of Conwell and Weisskopf, and Brooks and Herring whose theory is based on a scattering potential due to a stationary impurity, which is coulombic.

(iv) The results taking into account the effect of the oscillation of impurity ions are not sufficient to explain the deviations from the $T^{3/2}$ law.

It should be noted that the failure of using this effect to explain the deviation from the $T^{3/2}$ law observed in some non-polor semiconductors may be due to the following facts:

(i) The high temperature approximation may be inappropriate for non-degenerate semiconductors since at low temperatures, scattering by acoustic phonons through impurity oscillations becomes inelastic and can not be described using high temperature approximation.

(ii) High temperature approximation implies that the conduction electron energy is always greater than the interaction potential energy. However, there is a possibility that the conduction electrons are trapped by ionized impurities. In fact, such a possibility may become very signifficant, especially at low temperatures.

(iii) Direct interaction between phonons and oscillating impurities has been neglected in our calculation. this may also be very significant at low temperatures and with high impurity concentrations.

APPENDIX

(A) The Harmonic Oscillator and The Derivation of the General Form :

$$\langle \chi_{N_{\underset{\sim}{q}}} | (B_{\underset{\sim}{q}} + B^{+}_{\underset{\sim}{q}}) | \chi_{N_{\underset{\sim}{q}}} \rangle = \sum_{r=0}^{n} \frac{(2n)!\, 2^r}{2^n (r!)^2 (n-r)!} \cdot \frac{N_{\underset{\sim}{q}}!}{(N_{\underset{\sim}{q}} - r)!}$$

The Schrödinger equation for the harmonic oscillator is given by:

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \tfrac{1}{2} m \omega_q^2 x^2 \right] \chi_n(x) = E_n \chi_n(x) \qquad (A - 1)$$

where

$$E_n = \hbar \omega_q \left(n + \tfrac{1}{2} \right) \qquad (A - 2)$$

$$\chi_n(x) \equiv |n\rangle = \sqrt{\frac{\beta}{\pi^{\frac{1}{2}} 2^n\, n!}}\, H_n(\beta x) e^{-\frac{1}{2}\beta^2 x^2} \qquad (A - 3)$$

where $\chi_n(x)$ is normalized and $\beta = \sqrt{\frac{m\omega_q}{\hbar}}$.

Now we consider the following matrix element:

$$\langle n | \chi^p | m \rangle = \frac{\beta}{(\pi 2^{n+m} n! m!)^{\frac{1}{2}}} \int_{-\infty}^{\infty} \chi^p H_n(\beta x) H_m(\beta x) e^{-\beta^2 x^2} dx$$

$$= \frac{1}{\beta^p (\pi 2^{n+m} n! m!)^{\frac{1}{2}}} \int_{-\infty}^{\infty} \eta^p H_n(\eta) H_m(\eta) e^{-\eta^2} d\eta \qquad (\eta \equiv \beta x)$$

$$= \frac{2^{n-p}\, p!\, n!}{\beta^p (2^{n+m}\, n!m!)^{\frac{1}{2}}}\, S_p\,(n,m)$$

where use has been made of the following formula:

$$\int_{-\infty}^{\infty} \eta^p e^{-\eta^2} H_n(\eta) H_m(\eta) d\eta = \sqrt{\pi}\; 2^{n-p} p!\, n!\, S_p(n,m) \qquad (A - 4)$$

with

$$S_p\,(n,m) = \begin{cases} \displaystyle\sum_{\lambda=0}^{p/2} \sum_{\nu=0}^{2\lambda} \frac{2^{\nu}(n + 2\nu - 2\lambda)!\, \delta_{m,n+2\nu-2\lambda}}{\nu!(p/2 - \lambda)!\,(2\lambda - \nu)!(n + \nu - 2\lambda)!} & \text{(A - 4:a)} \\ \qquad \text{for } p = 2q \quad (q = 0,1,2,\cdots\cdots) & \\ \displaystyle\sum_{\lambda=0}^{(p-1)/2} \sum_{\nu=0}^{2\lambda+1} \frac{2^{\nu}(n+2\nu-2\lambda-1)!\, \delta_{m,n+2\nu-2\lambda-1}}{\nu!\{(p-1)/2 - \lambda\}!(2\lambda-\nu+1)!(n+\nu-2\lambda-1)!} & \text{(A - 4:b)} \\ \qquad \text{for } p = 2q + 1 \quad (q = 0,1,2,\cdots\cdots) & \end{cases}$$

Taking account of the fact that:

$m = n + 2\nu - 2\lambda$ when p is an even integer

and that :

$m = n + 2\nu - 2\lambda - 1$ when p is an odd integer,

the matrix element is

$$\langle n|\chi^p|m\rangle = \begin{cases} \dfrac{p!}{(2\beta)^p} \sum_{\lambda=0}^{p/2} \sum_{\nu=0}^{2\lambda} \dfrac{2^\lambda [n!(n+2\nu-2\lambda)!]^{\frac{1}{2}} \; \delta_{m,n+2\nu-2\lambda}}{\nu!(p/2-\lambda)!(2\lambda-\nu)!(n+\nu-2\lambda)!} & \text{(A - 5)} \\ \qquad\qquad \text{for even integers p} \\ \dfrac{p!}{(2\beta)^p} \sum_{\lambda=0}^{\frac{p-1}{2}} \sum_{\nu=0}^{2\lambda+1} \dfrac{2^{(\lambda+\frac{1}{2})} [n!(n+2\nu-2\lambda-1)!]^{\frac{1}{2}} \; \delta_{m,n+2\nu-2\lambda+1}}{\nu!(p/2-\lambda-\frac{1}{2})!(2\lambda-\nu+1)!(n+\nu-2\lambda-1)!} & \text{(A - 6)} \\ \qquad\qquad \text{for odd integers p} \end{cases}$$

For the case n=m (corresponding to energy conservation) the initial and the final states are the same, p(even) gives $\nu = \lambda$, but for p odd, m and n can never be equal. Thus only when p is even is energy conserved. Letting p = 2q (q = 0,1,2, ·····) in (A - 5), we have:

$$\langle n|\chi^{2q}|n\rangle = \frac{1}{(2\beta^2)^q} \sum_{\lambda=0}^{q} \frac{(2q)!\, 2^\lambda n!}{2^q(\lambda!)^2(q-\lambda)!(n-\lambda)!} \qquad \text{(A - 7)}$$

Now if we define:

$$\chi \equiv \sqrt{\frac{\hbar}{2\omega_q m}} \; (B_q + B_q^+) \qquad \text{(A - 8)}$$

$$P = i\sqrt{\frac{\hbar\omega_q m}{2}} \; (-B_q + B_q^+) \qquad \text{(A - 9)}$$

the Hamiltonian for the harmonic oscillator is:

$$\frac{p^2}{2m} + \tfrac{1}{2} m\omega_q x^2 \rightarrow \hbar\omega_q \left(B_{\underset{\sim}{q}}^{+} B_{\underset{\sim}{q}} + \tfrac{1}{2}\right) \qquad (A - 10)$$

which is exactly the same form given by (4-42) apart from the summation. (A - 10) expresses the Hamiltonian of the single harmonic oscillator with frequency ω_q. The operators $B_{\underset{\sim}{q}}$ and $B_{\underset{\sim}{q}}^{+}$ obey the commutation rules (4-45), (4-46) and (4-47). From (A-8), we have:

$$\langle n|x^p|m\rangle = \left(\sqrt{\frac{\hbar}{2\omega_q m}}\right)^p \langle n|(B_{\underset{\sim}{q}} + B_{\underset{\sim}{q}}^{+})^p|m\rangle \qquad (A - 11)$$

Replacing p by 2q for the case of energy conservation, we have:

$$\langle n|x^{2q}|n\rangle = \left(\sqrt{\frac{\hbar}{2\omega_q m}}\right)^{2q} \langle n|(B_{\underset{\sim}{q}} + B_{\underset{\sim}{q}}^{+})^{2q}|n\rangle$$

$$= \frac{1}{(2\beta^2)^q} \langle n|(B_{\underset{\sim}{q}} + B_{\underset{\sim}{q}}^{+})^{2q}|n\rangle \qquad (A - 12)$$

By comparing (A - 7) to (A - 12), the general form for elastic processes is:

$$\langle n|(B_{\underset{\sim}{q}} + B_{\underset{\sim}{q}}^{+})^{2q}|n\rangle = \sum_{\lambda=0}^{q} \frac{(2q)!\, 2^{\lambda} n!}{2^q (\lambda!)^2 (q-\lambda)!(n-\lambda)!} \qquad (A - 13)$$

i.e. by replacing n,q and λ by $N_{\underset{\sim}{q}}$, n and by r, respectively,

Thus :

$$\langle N_{\underset{\sim}{q}} | (B_{\underset{\sim}{q}} + B^{+}_{\underset{\sim}{q}})^{2n} | N_{\underset{\sim}{q}} \rangle = \sum_{r=0}^{n} \frac{(2n)!\, 2^r}{2^n (r!)^2 (n-r)!} \cdot \frac{N_{\underset{\sim}{q}}}{(N_{\underset{\sim}{q}} - r)!} \qquad (A - 14)$$

[Note: Derivation of (A - 4)]

The Hermite polynomials, $H_n(\eta)$, may be defined by the generating function:

$$g(\eta,z) = e^{-z^2+2z\eta} = \sum_{n=0}^{\infty} H_n(\eta) \frac{z^n}{n!} \qquad (i)$$

It follows from the generating function that:

$$\int_{-\infty}^{\infty} \eta^p e^{-\eta^2} g(\eta,z_1) g(m,z_2) d\eta$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{z_1^n z_2^m}{n!m!} \int_{-\infty}^{\infty} \eta^p e^{-\eta^2} H_n(\eta) H_m(\eta) d\eta$$

$$= \int_{-\infty}^{\infty} \eta^p e^{-\eta^2} e^{-z_1^2+2z_1\eta} e^{-z_2^2+2z_2\eta} d\eta$$

$$= e^{2z_1z_2} \int_{-\infty}^{\infty} \eta^p e^{-\{\eta - (z_1+z_2)\}^2} d\eta$$

Letting $u = \eta - (z_1 + z_2)$ we have:

$$\int_{-\infty}^{\infty} \eta^p e^{-\{\eta-(z_1+z_2)\}^2} d\eta = \int_{-\infty}^{\infty} \{u + (z_1 + z_2)\}^p e^{-u^2} du$$

so that:

$$\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{z_1^n z_2^m}{n\,m}\,I_p(n,m) = e^{2z_1z_2}\int_{-\infty}^{\infty}\{u+(z_1+z_2)\}^p e^{-u^2}\,du \qquad (ii)$$

where

$$I_p(n,m) \equiv \int_{-\infty}^{\infty}\eta^p e^{-\eta^2} H_n(\eta)H_m(\eta)d\eta \qquad (iii)$$

(a) Case p = 2q = even integers (q = 0,1,2,·····)

$$\{u+(z_1+z_2)\}^p \to \{u+(z_1+z_2)\}^{2q}$$

$$= \sum_{s=0}^{2q}\binom{2q}{s}\,u^{2q-s}(z_1+z_2)^s$$

$$= \sum_{s=0}^{2q}\frac{(2q)!}{s!(2q-s)!}u^{2q-s}(z_1+z_2)^s$$

Since e^{-u^2} is an even function, only even integers s, i.e. $s = 2\lambda$ ($\lambda = 0,1,2,\cdots\cdots$) contribute to the integral in (ii). Hence putting $s = 2\lambda$, we have

$$\{u+(z_1+z_2)\}^{2q} = \sum_{s=0}^{q}\frac{(2q)!}{(2\lambda)!\{2(q-\lambda)\}!}\,u^{2(q-\lambda)}\,(z_1+z_2)^{2\lambda}$$

so that:

$$e^{2z_1z_2} \int_{-\infty}^{\infty} \{u + (z_1+z_2)\}^{2q} e^{-u^2} du$$

$$= e^{2z_1z_2} \sum_{\lambda=0}^{q} \frac{(2q)!\,(z_1+z_2)^{2\lambda}}{(2\lambda)!\,\{2(q-\lambda)\}!} \int_{-\infty}^{\infty} u^{2(q-\lambda)} e^{-u^2} du$$

$$= e^{2z_1z_2} \sum_{\lambda=0}^{q} \frac{\sqrt{\pi}\,(2q)!\,(z_1+z_2)^{2\lambda}}{2^{2(q-\lambda)}(2\lambda)!(q-\lambda)!}$$

where use has been made of the following formula:

$$\int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx = \frac{(2n)!}{2^{2n}\,n!} \sqrt{\frac{\pi}{\alpha^{2n+1}}} \qquad \text{(iv)}$$

(n: positive integers)

Since:

$$e^{2z_1z_2} = \sum_{n'}^{\infty} \frac{(2z_1z_2)^{n'}}{n'!}$$

and

$$(z_1 + z_2)^{2\lambda} = \sum_{\nu=0}^{2\lambda} \binom{2\lambda}{\nu} z_1^{2\lambda-\nu} z_2^{\nu}$$

$$= \sum_{\nu=0}^{2\lambda} \frac{(2\lambda)!}{\nu!\,(2\lambda-\nu)!} z_1^{2\lambda-\nu} z_2^{\nu}$$

we have:

$$e^{2z_1z_2} \sum_{\lambda=0}^{q} \frac{\sqrt{\pi}\,(2q)!(z_1+z_2)^{2\lambda}}{2^{2(q-\lambda)}\,(2\lambda)!(q-\lambda)!}$$

$$= \sqrt{\pi}\,(2q)! \sum_{n'=0}^{\infty} \sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda} \frac{2^{n'}}{n'!} \frac{z_1^{\,n'+2\lambda-\nu} z_2^{\,n'+\nu}}{2^{2(q-\lambda)}(q-\lambda)!\,\nu!(2\lambda-\nu)!}$$

$$= \sqrt{\pi}\,(2q)! \sum_{n'=0}^{\infty} \sum_{m=0}^{\infty} \left[\sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda} \frac{2^{n'}}{n'!} \frac{z_1^{\,n'+2\lambda-\nu} z_2^{\,m}\, \delta_{m,n'+\nu}}{2^{2(q-\lambda)}(q-\lambda)!\,\nu!(2\lambda-\nu)!} \right]$$

Putting $n'+2\lambda-\nu = n$, i.e. $n' = n+\nu-2\lambda$

$$= \sqrt{\pi}\,(2q)! \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left\{ \sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda} \frac{2^{n+\nu-2\lambda} z_1^{\,n} z_2^{\,m}\, \delta_{m,n+2\nu-2\lambda}}{2^{2(q-\lambda)}(q-\lambda)!\,\nu!(2\lambda-\nu)!\,(n+\nu-2\lambda)!} \right\}$$

Hence we have:

$$\sum_{n=0}^{\infty} \sum_{m=0}^{\infty} z_1^{\,n} z_2^{\,m} \frac{I_{2q}(n,m)}{n!m!}$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} z_1^{\,n} z_2^{\,m} \left[\sqrt{\pi}\,(2q)! \sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda} \frac{2^{n-2q+\nu}\, \delta_{m,n+2\nu-2\lambda}}{(q-\lambda)!\,\nu!(2\lambda-\nu)!\,(n+\nu-2\lambda)!} \right]$$

By equating the coefficients of $z_1^n z_2^m$ on both sides, we have the following formula:

$$I_{2q}(n,m) = \sqrt{\pi}\, 2^{n-2q}\, (2q)!\, n! \sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda} \frac{2^{\nu}(n+2\nu-2\lambda)!\,\delta_{m,n+2\nu-2\lambda}}{(q-\lambda)!\,\nu!\,(2\lambda-\nu)!\,(n+\nu-2\lambda)!} \qquad (v)$$

(b) Case $p = 2q+1$ = odd integers ($q = 0,1,2,\cdots\cdots$)

$$\{u + (z_1+z_2)\}^p \to \{u + (z_1+z_2)\}^{2q+1}$$

$$= \sum_{s=0}^{2q+1} \binom{2q+1}{s} u^{2q-s+1}(z_1+z_2)^s$$

$$= \sum_{s=0}^{2q+1} \frac{(2q+1)!}{s!(2q-s+1)!}\, u^{2q-s+1}(z_1+z_2)^s$$

Since e^{-u^2} is an even function, only odd integers s, i.e. $s = 2\lambda+1$ ($\lambda = 0,1,2,\cdots\cdots$) contribute to the integral in (ii). Hence putting $s = 2\lambda+1$, we have:

$$\{u + (z_1+z_2)\}^{2q+1} = \sum_{s=0}^{q} \frac{(2q+1)!}{(2\lambda+1)!\,\{2(q-\lambda)\}!}\, u^{2(q-\lambda)}(z_1+z_2)^{2\lambda+1}$$

so that:

$$e^{2z_1z_2} \int_{-\infty}^{\infty} \{u + (z_1+z_2)\}^{2q+1} \, e^{-u^2} \, du$$

$$= e^{2z_1z_2} \sum_{\lambda=0}^{q} \frac{(2q+1)!\,(z_1+z_2)^{2\lambda+1}}{(2\lambda+1)!\,\{2(q-\lambda)\}!} \int_{-\infty}^{\infty} u^{2(q-\lambda)} \, e^{-u^2} \, du$$

$$= e^{2z_1z_2} \sum_{\lambda=0}^{q} \frac{\sqrt{\pi}(2q+1)!\,(z_1+z_2)^{2\lambda+1}}{2^{2(q-\lambda)}\,(2\lambda+1)!\,(q-\lambda)!}$$

where use has been made of (iv).

Since:

$$e^{2z_1z_2} = \sum_{n'=0}^{\infty} \frac{(2z_1z_2)^{n'}}{n'!}$$

and

$$(z_1+z_2)^{2\lambda+1} = \sum_{\nu=0}^{2\lambda+1} \binom{2\lambda+1}{\nu} z_1^{\,2\lambda-\nu+1} \, z_2^{\,\nu}$$

$$= \sum_{\nu}^{2\lambda+1} \frac{(2\lambda+1)!}{\nu!\,(2\lambda-\nu+1)!} z_1^{\,2\lambda-\nu+1} \, z_2^{\,\nu}$$

we have:

$$e^{2z_1z_2} \sum_{\lambda=0}^{q} \frac{\sqrt{\pi}\,(2q+1)!\,(z_1+z_2)^{2\lambda+1}}{2^{2(q-\lambda)}(2\lambda+1)!\,(q-\lambda)!}$$

$$= \sqrt{\pi}\,(2q+1)! \sum_{n'=0}^{\infty} \sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda+1} \frac{2^{n'}}{n'!} \cdot \frac{z_1^{\,n'+2\lambda-\nu+1}\, z_2^{\,n'+\nu}}{2^{2(q-\lambda)}(q-\lambda)!\,\nu!\,(2\lambda-\nu+1)!}$$

$$= \sqrt{\pi}\,(2q+1)! \sum_{n'=0}^{\infty} \sum_{m=0}^{\infty} \left[\sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda+1} \frac{2^{n'}}{n'!} \cdot \frac{z_1^{\,n'+2\lambda-\nu+1}\, z_2^{\,m}\, \delta_{m,n'+\nu}}{2^{2(q-\lambda)}(q-\lambda)!\,\nu!\,(2\lambda-\nu+1)!} \right]$$

Putting $n'+2\lambda-\nu+1 = n$; i.e. $n' = n+\nu-2\lambda-1$

$$= \sqrt{\pi}\,(2q+1)! \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left[\sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda+1} \frac{2^{n+\nu-2\lambda-1} z_1^{\,n}\, z_2^{\,m}\, \delta_{m,n+2\nu-2\lambda-1}}{2^{2(q-\lambda)}(q-\lambda)!\,\nu!\,(2\lambda-\nu+1)!\,(n+\nu-2\lambda+1)!} \right]$$

Hence we have:

$$\sum_{n=0}^{\infty} \sum_{m=0}^{\infty} z_1^{\,n}\, z_2^{\,m}\, \frac{I_{2q+1}(n,m)}{n!\,m!}$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} z_1^{\,n} z_2^{\,m} \left[\sqrt{\pi}\,(2q+1)! \sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda+1} \frac{2^{n-2q+\nu-1}\, \delta_{m,n+2\nu-2\lambda-1}}{(q-\lambda)!\,\nu!\,(2\lambda-\nu+1)!\,(n+\nu-2\lambda+1)!} \right]$$

from which we have the following formula:

$$I_{2q+1}(n,m) = \sqrt{\pi}\, 2^{n-(2q+1)}\, (2q+1)!\, n! \sum_{\lambda=0}^{q} \sum_{\nu=0}^{2\lambda+1} \frac{2^{\nu}(n+2\nu-2\lambda-1)!\,\delta_{m,n+2\nu-2\lambda-1}}{(q-\lambda)!\,\nu!\,(2\lambda-\nu+1)!\,(n+\nu-2\lambda-1)!} \qquad \text{(vi)}$$

From the results (v) and (vi) we have the formula (A - 4).

(B) Thermal Equilibrium Situation:

If the system is at the equilibrium, we can replace $N_{\underset{\sim}{q}}$ for phonons and $f(\underset{\sim}{k})$ for electrons in (9-3) by their equilibrium distribution functions, i.e.,

$$N_{\underset{\sim}{q}} = \frac{1}{e^{\beta\hbar\omega_q} - 1} \qquad \text{and} \qquad f^o(\underset{\sim}{k}) = \frac{1}{e^{\beta(E_{\underset{\sim}{k}}-\mu)} + 1}$$

respectively. Noting the property of the δ-function, i.e., $\delta(x) = \delta(-x)$, the first and the fourth terms in (9-3) are then:

$$\{(N_{\underset{\sim}{q}} + 1)f^o(\underset{\sim}{k}')(1 - f^o(\underset{\sim}{k})) - N_{\underset{\sim}{q}} f^o(\underset{\sim}{k})(1 - f^o(\underset{\sim}{k}'))\}\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} - \hbar\omega_q)$$

$$= \{(f^o(\underset{\sim}{k}') - f^o(\underset{\sim}{k}))N_{\underset{\sim}{q}} + f^o(\underset{\sim}{k}')(1 - f^o(\underset{\sim}{k}))\}\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} - \hbar\omega_q)$$

$$= \frac{e^{\beta(E_{\underset{\sim}{k}}+\hbar\omega_q-\mu)} - e^{\beta(E_{\underset{\sim}{k}'}-\mu)}}{(e^{\beta(E_{\underset{\sim}{k}'}-\mu)} + 1)(e^{\beta(E_{\underset{\sim}{k}}-\mu)} + 1)(e^{\beta\hbar\omega_q} - 1)}\delta(E_{\underset{\sim}{k}'} - E_{\underset{\sim}{k}} - \hbar\omega_q)$$

where due to the δ-function we can replace $E_{\underset{\sim}{k}} + \hbar\omega_q$ by $E_{\underset{\sim}{k}'}$. The above result, therefore, vanishes. In the same way we can prove that the second and the third terms in (9-3) also vanish at thermal equilibrium. Hence the collision term, (9-3), goes to zero and both (9-5:a) and (9-5:b) hold.

(C) Derivation of the Linearized Boltzmann's Equation:

By use of (10-6) and noting the equality (9-5:a), the first and the fourth terms in (9-3) are:

$$\left[(N_{\underset{\sim}{q}}+1)f(\underset{\sim}{k}')(1-f(\underset{\sim}{k})) - N_{\underset{\sim}{q}}f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))\right]\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)$$

$$= \left[(N_{\underset{\sim}{q}}+1)\{f^\circ(\underset{\sim}{k}')-\Phi(\underset{\sim}{k}')\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}'}}\}\{1-f^\circ(\underset{\sim}{k})+\Phi(\underset{\sim}{k})\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}}}\}\right.$$

$$\left.-N_{\underset{\sim}{q}}\{f^\circ(\underset{\sim}{k})-\Phi(\underset{\sim}{k})\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}}}\}\{1-f^\circ(\underset{\sim}{k}')+\Phi(\underset{\sim}{k}')\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}'}}\}\right]\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)$$

$$= \left[\underline{(N_{\underset{\sim}{q}}+1)f^\circ(\underset{\sim}{k}')(1-f^\circ(\underset{\sim}{k}))}+(N_{\underset{\sim}{q}}+1)f^\circ(\underset{\sim}{k}')\Phi(\underset{\sim}{k})\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}}}\right.$$

$$-(N_{\underset{\sim}{q}}+1)(1-f^\circ(\underset{\sim}{k}))\Phi(\underset{\sim}{k}')\frac{\partial f}{\partial E_{\underset{\sim}{k}'}} - \cancel{(N_{\underset{\sim}{q}}+1)\Phi(\underset{\sim}{k})\Phi(\underset{\sim}{k}')\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}}}\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}'}}}\ \text{omit}$$

$$\underline{-N_{\underset{\sim}{q}}f^\circ(\underset{\sim}{k})(1-f^\circ(\underset{\sim}{k}'))}-N_{\underset{\sim}{q}}f^\circ(\underset{\sim}{k})\Phi(\underset{\sim}{k}')\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}'}}$$

$$\left.+N_{\underset{\sim}{q}}(1-f^\circ(\underset{\sim}{k}'))\Phi(\underset{\sim}{k})\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}}} \cancel{+N_{\underset{\sim}{q}}\Phi(\underset{\sim}{k})\Phi(\underset{\sim}{k}')\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}}}\frac{\partial f^\circ}{\partial E_{\underset{\sim}{k}'}}}\ \text{omit}\right]\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)$$

$$= \left[(N_{\underset{\sim}{q}}+1)\{f^{o}(\underset{\sim}{k}')\Phi(\underset{\sim}{k})\frac{\partial f^{o}}{\partial E_{\underset{\sim}{k}}} - (1-f^{o}(\underset{\sim}{k}))\Phi(\underset{\sim}{k}')\frac{\partial f^{o}}{\partial E_{\underset{\sim}{k}'}}\}\right.$$

$$\left. -N_{\underset{\sim}{q}}\{f^{o}(\underset{\sim}{k})\Phi(\underset{\sim}{k}')\frac{\partial f^{o}}{\partial E_{\underset{\sim}{k}'}} - (1-f^{o}(\underset{\sim}{k}'))\Phi(\underset{\sim}{k})\frac{\partial f^{o}}{\partial E_{\underset{\sim}{k}}}\}\right] \delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_{q})$$

where the terms with ------ have been canceled each other due to (9-5:a) and the terms of Φ^2 have been omitted since we are cosidering only up to the first order power of $\underset{\sim}{E}$ (electric field).

Substituting (10-5) into the above equation and noting (9-5:a), the above equation becomes:

$$\left[(N_{\underset{\sim}{q}}+1)f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))-N_{\underset{\sim}{q}}f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))\right] \delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_{q})$$

$$= \beta\left[N_{\underset{\sim}{q}}f^{o}(\underset{\sim}{k})(1-f^{o}(\underset{\sim}{k}'))\Phi(\underset{\sim}{k}')f^{o}(\underset{\sim}{k}')-N_{\underset{\sim}{q}}f^{o}(\underset{\sim}{k})(1-f^{o}(\underset{\sim}{k}'))\Phi(\underset{\sim}{k})(1-f^{o}(\underset{\sim}{k}))\right.$$

$$\left. +(N_{\underset{\sim}{q}}+1)f^{o}(\underset{\sim}{k}')(1-f^{o}(\underset{\sim}{k}))\Phi(\underset{\sim}{k}')(1-f^{o}(\underset{\sim}{k}'))-(N_{\underset{\sim}{q}}+1)f^{o}(\underset{\sim}{k}')(1-f^{o}(\underset{\sim}{k}))\Phi(\underset{\sim}{k})f^{o}(\underset{\sim}{k})\right]$$

$$\times \delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_{q})$$

$$= \beta N_{\underset{\sim}{q}}f^{o}(\underset{\sim}{k})(1-f^{o}(\underset{\sim}{k}'))(\Phi(\underset{\sim}{k}')-\Phi(\underset{\sim}{k}))\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_{q}) \qquad \text{(C-1)}$$

Similarly, by use of (10-6) and noting the equality (9-5:b), the second and the third terms in (9-3) are:

$$\left[N_{\underset{\sim}{q}} f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))-(N_{\underset{\sim}{q}}+1)f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))\right]\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)$$

$$= \beta N_{\underset{\sim}{q}} f^{o}(\underset{\sim}{k}')(1-f^{o}(\underset{\sim}{k}))(\Phi(\underset{\sim}{k}')-\Phi(\underset{\sim}{k}))\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q) \qquad \text{(C-2)}$$

where use has been made of (10-5) and the terms of Φ^2 have been omitted.

From (C-1) and (C-2) there results:

$$\left[\{(N_{\underset{\sim}{q}}+1)f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))-N_{\underset{\sim}{q}} f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))\}\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)\right.$$

$$\left.+\{N_{\underset{\sim}{q}} f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))-(N_{\underset{\sim}{q}}+1)f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))\}\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)\right]$$

$$= \beta N_{\underset{\sim}{q}}\left[f^{o}(\underset{\sim}{k})(1-f^{o}(\underset{\sim}{k}'))\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q) + f^{o}(\underset{\sim}{k}')(1-f^{o}(\underset{\sim}{k}))\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)\right]$$

$$\times\left[\Phi(\underset{\sim}{k}') - \Phi(\underset{\sim}{k})\right] \qquad \text{(C-3)}$$

Replacing the square bracket in (9-3) by (C-3) leads to the collision term (10-8), from which the Linearized Boltzmann's equation follows.

(D) Derivation of τ_p ; Electron Scattering from Lattice Oscillation:

(i) Electron-Lattice Interaction

We consider the interaction between a conduction electron and the acoustic vibrations of atoms, which make up the lattice field. If the lattice is regarded as continuum (see Chap. 4), one expects the interaction between an electron at $\underset{\sim}{r}$ and a density wave at $\underset{\sim}{R}$ to be proportional to the product:

$$|\psi(r)|^2 \underset{\sim}{\nabla}\cdot\underset{\sim}{u}(\underset{\sim}{R},t) \qquad \text{(D-1)}$$

where $|\psi|^2$ is the probability density of the conduction electrons and $\underset{\sim}{\nabla}\cdot\underset{\sim}{u}$ is the volume change in the medium. The total interaction between the conduction electron and the lattice oscillations is then given by:

$$H_{int} = C\int_{\underset{\sim}{R}} |\psi(r)|^2 \, \underset{\sim}{\nabla}\cdot\underset{\sim}{u}(\underset{\sim}{R},t)d\underset{\sim}{R}^3 \qquad \text{(D-2)}$$

where C is a deformation potential constant (an electro-phonon coupling constant) having the dimensions of energy and is determined by experiments. (D-2) shows the energy change due to the volume change (or density change) of the medium.

Suppose that:

$$|\psi(r)|^2 = \delta(\underset{\sim}{r} - \underset{\sim}{R}) \qquad \text{(D-3)}$$

then (D-2) becomes:

$$H_{int} = C \, \underset{\sim}{\nabla} \cdot \underset{\sim}{\eta}(\underset{\sim}{r},t) \tag{D-4}$$

Using the displacement vector given by (4-43), (D-4) becomes:

$$H_{int} = - C\sqrt{\frac{\hbar}{2\rho_o V_o S_o}} \sum_{\underset{\sim}{q}} q^{\frac{1}{2}} \left[B_{\underset{\sim}{q}} \, e^{i\underset{\sim}{q}\cdot\underset{\sim}{r}} - B^{+}_{\underset{\sim}{q}} \, e^{-i\underset{\sim}{q}\cdot\underset{\sim}{r}} \right] \tag{D-5}$$

where the sound speed S_o is given by:

$$S_o = \sqrt{\frac{1}{K_o \rho_o}} \tag{D-6}$$

where K_o is the compressibility and ρ_o is the density of the medium. We note here that $B_{\underset{\sim}{q}}$ and $B^{+}_{\underset{\sim}{q}}$ are, respectively, phonon destruction and creation operators. Since the minus sign in (D-5) comes from a trivial phase factor, $e^{i\pi}$, we can simply write (D-5) as:

$$H_{int} = C\sqrt{\frac{\hbar}{2\rho_o V_o S_o}} \sum_{\underset{\sim}{q}} q^{\frac{1}{2}} \left(B_{\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{r}} - B^{+}_{\underset{\sim}{q}} e^{-i\underset{\sim}{q}\cdot\underset{\sim}{r}} \right) \tag{D-7}$$

(ii) The Basic Hamiltonian for Intrinsic Semiconductors

The Hamiltonian of the system for intrinsic semiconductors is:

$$H = H_{lattice} + H_{electron} + H_{int} \tag{D-8}$$

where $H_{lattice}$, $H_{electron}$ and H_{int} are given by (5-2:a), (5-2:b) and (D-7), respectively. Since $H_{lattice}$ and $H_{electron}$ are independent each other, the wave function of the unperturbed system ($H_{lattice} + H_{electron}$) is given by (6-2).

(iii) Matrix Elements for Scattering

The rate at which a conduction electron in a state $\underset{\sim}{k}$ is scattered into another state $\underset{\sim}{k}'$ by a lattice oscillation is determined by the matrix element:

$$\langle \underset{\sim}{n}', \underset{\sim}{k}' | H_{int} | \underset{\sim}{n}, \underset{\sim}{k} \rangle = C\sqrt{\frac{\hbar}{2\rho_o V_o S_o}} \sum_{\underset{\sim}{q}} q^{\frac{1}{2}} \left[\langle \chi_{N'_{\underset{\sim}{q}}} | B_{\underset{\sim}{q}} | \chi_{N_{\underset{\sim}{q}}} \rangle \frac{1}{V_o} \int_{\underset{\sim}{r}} e^{i(\underset{\sim}{q}-\underset{\sim}{k}'-\underset{\sim}{k})\cdot\underset{\sim}{r}} d\underset{\sim}{r}^3 \right.$$

$$\left. - \langle \chi_{N'_{\underset{\sim}{q}}} | B^{+}_{\underset{\sim}{q}} | \chi_{N_{\underset{\sim}{q}}} \rangle \frac{1}{V_o} \int_{\underset{\sim}{r}} e^{-i(\underset{\sim}{q}+\underset{\sim}{k}'-\underset{\sim}{k})\cdot\underset{\sim}{r}} d\underset{\sim}{r}^3 \right] \qquad \text{(D-9)}$$

where use has been made of (6-2).

Since:

$$\int_{\underset{\sim}{r}} e^{i(\underset{\sim}{k}-\underset{\sim}{k}'\pm\underset{\sim}{q})\cdot\underset{\sim}{r}} d\underset{\sim}{r}^3 = V_o \delta_{\underset{\sim}{k}', \underset{\sim}{k}\pm\underset{\sim}{q}} \qquad \text{(D-10)}$$

(D-9) becomes:

$$\langle \underset{\sim}{n}', \underset{\sim}{k}' | H_{int} | \underset{\sim}{n}, \underset{\sim}{k} \rangle = C \sqrt{\frac{\hbar}{2\rho_o V_o S_o}} \sum_{\underset{\sim}{q}} q^{\frac{1}{2}} \Big[\langle \chi_{N'_{\underset{\sim}{q}}} | B_{\underset{\sim}{q}} | \chi_{N_{\underset{\sim}{q}}} \rangle \delta_{\underset{\sim}{k}', \underset{\sim}{k}+\underset{\sim}{q}}$$

$$- \langle \chi_{N'_{\underset{\sim}{q}}} | B^{+}_{N_{\underset{\sim}{q}}} | \chi_{N_{\underset{\sim}{q}}} \rangle \delta_{\underset{\sim}{k}', \underset{\sim}{k}-\underset{\sim}{q}} \Big]$$

$$= C \sqrt{\frac{\hbar}{2\rho_o V_o S_o}} |\underset{\sim}{k}' - \underset{\sim}{k}|^{\frac{1}{2}} \Big[\langle \chi_{N'_{\underset{\sim}{k}'-\underset{\sim}{k}}} | B_{\underset{\sim}{k}'-\underset{\sim}{k}} | \chi_{N_{\underset{\sim}{k}'-\underset{\sim}{k}}} \rangle$$

$$- \langle \chi_{N'_{-(\underset{\sim}{k}'-\underset{\sim}{k})}} | B^{+}_{-(\underset{\sim}{k}'-\underset{\sim}{k})} | \chi_{N_{-(\underset{\sim}{k}'-\underset{\sim}{k})}} \rangle \Big] \quad \text{(D-11)}$$

We see that the transition $\underset{\sim}{k} \to \underset{\sim}{k}'$ of a conduction electron and the simultaneous transition $N_{\underset{\sim}{q}} \to N_{\underset{\sim}{q}} \pm 1$ of the $\underset{\sim}{q}^{th}$ lattice mode can occur only when (D-10) is satisfied; i.e.,

$$\underset{\sim}{k}' - \underset{\sim}{k} \pm \underset{\sim}{q} = 0 \quad \text{(D-12)}$$

which ensures the momentum conservation.

Noting (D-12) and the orthogonality of the lattice wave function, (D-11) is reduced to:

$$\langle N_{\underset{\sim}{q}}-1, \underset{\sim}{k}' | H_{int} | N_{\underset{\sim}{q}}, \underset{\sim}{k} \rangle = C \sqrt{\frac{\hbar q}{2\rho_o V_o S_o}} N^{\frac{1}{2}}_{\underset{\sim}{q}} \quad \text{(D-13:a)}$$

$$\langle N_{\underset{\sim}{q}}+1, \underset{\sim}{k}' | H_{int} | N_{\underset{\sim}{q}}, \underset{\sim}{k} \rangle = C \sqrt{\frac{\hbar q}{2\rho_o V_o S_o}} (N_{\underset{\sim}{q}}+1)^{\frac{1}{2}} \quad \text{(D-13:b)}$$

where use has been made of (4-48) and (4-49). Here (D-13:a) and (D-13:b) correspond to the phonon absorption and the phonon emission processes, respectively.

(iv) Transition Probability

From (D-13:a,b), the transition probability for one-phonon processes is:

$$P_{\underset{\sim}{n}\underset{\sim}{k}\to\underset{\sim}{n}'\underset{\sim}{k}'} = \frac{\pi C^2}{\rho_o V_o S_o} q\left[N_{\underset{\sim}{q}}\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q) + (N_{\underset{\sim}{q}}+1)\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)\right]$$

$$= P^A(\underset{\sim}{k},\underset{\sim}{k}'=\underset{\sim}{k}+\underset{\sim}{q}) + P^E(\underset{\sim}{k},\underset{\sim}{k}'=\underset{\sim}{k}-\underset{\sim}{q}) \qquad \text{(D-14)}$$

where:

$$P^A(\underset{\sim}{k},\underset{\sim}{k}') = \frac{\pi C^2}{\rho_o V_o S_o} q\, N_{\underset{\sim}{q}}\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q) \qquad \text{(D-14:a)}$$

and

$$P^E(\underset{\sim}{k},\underset{\sim}{k}') = \frac{\pi C^2}{\rho_o V_o S_o} q(N_{\underset{\sim}{q}}+1)\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q) \qquad \text{(D-14:b)}$$

are the transition probability for the phonon absorption and the phonon emission processes, respectively.

(v) Collision Term

Using (D-14) and taking into account of the principle of micro-reversibility and of the probability of electron occupations, $f(\underset{\sim}{k})(1-f(\underset{\sim}{k}))$, i.e., the probability that the initial state $\underset{\sim}{k}$ is occupied and the final state $\underset{\sim}{k}'$ is unoccupied, the collision term in the Boltzmann equation is:

$$\left(\frac{\partial f(\underset{\sim}{k})}{\partial t}\right)_{\text{collision}} = \sum_{\underset{\sim}{k}'}\Big[\, P(\underset{\sim}{k}',\underset{\sim}{k})f(\underset{\sim}{k}')\{1-f(\underset{\sim}{k})\} - P(\underset{\sim}{k},\underset{\sim}{k}')f(\underset{\sim}{k})\{1-f(\underset{\sim}{k}')\}\Big]$$

$$= \sum_{\underset{\sim}{k}'}\Big[\, P^{E}(\underset{\sim}{k}',\underset{\sim}{k})f(\underset{\sim}{k}')(1-f(\underset{\sim}{k})) + P^{A}(\underset{\sim}{k}',\underset{\sim}{k})f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))$$

$$- P^{E}(\underset{\sim}{k},\underset{\sim}{k}')f(\underset{\sim}{k})(1-f(\underset{\sim}{k}')) - P^{A}(\underset{\sim}{k},\underset{\sim}{k}')f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))\Big] \qquad \text{(D-15)}$$

where we may replace the sum over all the final states, $\underset{\sim}{k}'$, by an integral using the density of states function (7-15). We note here that each term in (D-15) corresponds to its diagram given by Fig. I. Using (D-14:a,b) and (7-15), we have (D-15) as:

$$\left(\frac{\partial f(\underset{\sim}{k})}{\partial t}\right)_{\text{collision}} = \frac{c^2}{8\pi^2 \rho_o V_o S_o}\int_{\underset{\sim}{k}'} q\Big[(N_{\underset{\sim}{q}}+1)f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))\delta(E_{\underset{\sim}{k}}-E_{\underset{\sim}{k}'}+\hbar\omega_{\underset{\sim}{q}})$$

$$+ N_{\underset{\sim}{q}} f(\underset{\sim}{k}')(1-f(\underset{\sim}{k}))\delta(E_{\underset{\sim}{k}}-E_{\underset{\sim}{k}'}-\hbar\omega_{\underset{\sim}{q}}) - (N_{\underset{\sim}{q}}+1)f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))$$

$$\times \delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q) - N_{\underset{\sim}{q}} f(\underset{\sim}{k})(1-f(\underset{\sim}{k}'))\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)\Big] d\underset{\sim}{k}'^3 \qquad \text{(D-16)}$$

(D-16) is the change in the distribution function, $f(\underset{\sim}{k})$, due to the interaction between the conduction electrons and the lattice.

(vi) Linearized Boltzmann Equation

Derivation of the Linearized Boltzmann equation is exactly the same as that given in Chap.10. Noting the terms in the square brackets in (9-3) and (D-16) are exactly the same, and substituting (10-6) into (D-16), we have the Linearized Boltzmann equation as:

$$\frac{c^2\beta}{8\pi^2\rho_o S_o}\int_{\underset{\sim}{k}'} qN_{\underset{\sim}{q}}\Big[\Phi(\underset{\sim}{k}') - \Phi(\underset{\sim}{k})\Big]\Psi d\underset{\sim}{k}'^3 = \frac{e\underset{\sim}{E}}{\hbar}\cdot\frac{\partial f^o(\underset{\sim}{k})}{\partial \underset{\sim}{k}} \qquad \text{(D-17)}$$

where Ψ and Φ are given by (10-10) and (10-7), respectively, and $\beta = (k_B T_e)^{-1}$. (D-17) is the basic equation to determine τ.

For non-degenerate intrinsic semiconductors we can use (11-1) for conduction electrons. We, therefore, can replace the square brackets in (10-10) by unity. Assuming $\underset{\sim}{E} = (0,0,E_z)$, (D-17) becomes:

$$\frac{c^2\beta}{8\pi^2\rho_o S_o}\int_{\underset{\sim}{k}'} qN_{\underset{\sim}{q}}\Big[k_z'\tau(\underset{\sim}{k}') - k_z\tau(\underset{\sim}{k})\Big]\Big[f^o(\underset{\sim}{k})\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}-\hbar\omega_q)$$

$$+ f^o(\underset{\sim}{k}')\delta(E_{\underset{\sim}{k}'}-E_{\underset{\sim}{k}}+\hbar\omega_q)\Big] d\underset{\sim}{k}'^3 = \frac{m^*}{\hbar^2}\cdot\frac{\partial f^o(\underset{\sim}{k})}{\partial k_z} \qquad \text{(D-18)}$$

(vii) Relaxation Time for Momentum Transfer

Noting the integral over the final states, $\underset{\sim}{k}'$, is exactly the same form as (11-3), (D-18) becomes:

$$-\frac{C^2(2m^*)^{\frac{1}{2}}\, qk_z}{2\pi\rho_o S_o \hbar}\,\tau(\underset{\sim}{k})N_{\underset{\sim}{q}}\left[(E_{\underset{\sim}{k}}+\hbar\omega_q)^{\frac{1}{2}}f^o(E_{\underset{\sim}{k}})+(E_{\underset{\sim}{k}}-\hbar\omega_q)^{\frac{1}{2}}f^o(E_{\underset{\sim}{k}}-\hbar\omega_q)\right]=\frac{\partial f^o(E_k)}{\partial k_z} \qquad \text{(D-19)}$$

From (11-5), (11-6), (11-7) and (11-9) for the high temperature approximation and from (D-19), we have the reciprocal of relaxation time due to the electron -lattice interaction; i.e., electron-phonon scattering, as:

$$\frac{1}{\tau_p}=\frac{1}{2\pi}\cdot\frac{(2m^*)^{3/2}}{\hbar^4}\cdot\frac{k_B T}{\rho_o S_o^2}\,C^2\,E_{\underset{\sim}{k}}^{\frac{1}{2}} \qquad \text{(D-20)}$$

We note here that (D-20) is valid for $T > 1\ ^oK$.

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